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CALCULATION OF ENGINE PERFORMANCE USING AMMONIA FUEL. III. BRAYTON CYCLE

Henry K. Newhall

University of California Berkeley, California

December 1965

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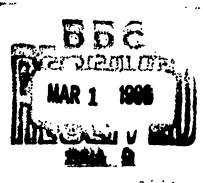
USING AMMONIA FUEL

III. BRAYTON CYCLE

by

Henry K. Newhall

Report No. TS-65-6 Contract DA-04-200-AMC-791(X) December 1965



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CALCULATION OF ENGINE PERFORMANCE USING AMMONIA FUEL 111. BRAYTON CYCLE

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by

Henry K. Newhall

Technical Report No. 4

Under Contract
DA-04-200-AMC-791 (X) Ammonia Fuel
Army Material Command
R & D Directorate
Chemistry and Materials Branch

Project Director E. S. Starkman

December 1965

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SUMMARY

The performance of ammonia as a fuel for gas turbine application has been theoretically predicted. Regenerative and non-regenerative Brayton cycles were employed as theoretical models, and combustion products were treated as a chemical equilibrium reactive system. All calculations were carried out by programs developed for use on an IBM 7094 digital computer.

The following conclusions are based upon the theoretically predicted results:

- 1) Ammonia can yield power output up to 10% greater than that for hydrocarbon fuels operating under the same conditions of limited turbine inlet temperature.
- 2) Thermal efficiencies for ammonia should range up to 10% higher than those for hydrocarbon fuels.
- 3) Specific fuel consumption for ammonia is predicted to exceed by 2-1/2 to 3 times that for hydrocarbon fuels.

-

CALCULATION OF ENGINE PERFORMANCE USING AMMONIA FUEL III. BRAYTON CYCLE

INTRODUCTION

This is the fourth report in a series of theoretical studies dealing with combustion engine cycles using ammonia fuel. The first report (1) presented the chemical equilibrium properties of ammonia-air combustion products and method of calculation. The second and third reports (2)(3) were concerned respectively with the predicted theoretical performance of spark ignition (Otto cycle) and compression ignition (Diesel cycle) engines with ammonia as fuel. This report presents the theoretically predicted performance of ammonia as a gas turbine fuel (Brayton cycle).

In its simplest form, operation of the gas turbine is represented thermodynamically by the theoretical Brayton cycle shown in Figure 1. In terms of elementary processes, this cycle is characterized by isentropic compression of air charge, 1-2, constant pressure heat addition (combustion), 2-3, and isentropic expansion with production of useful shaft work, 3-4.

For the purpose of a very simple analysis, the working fluid of the Brayton cycle might be treated as a pure substance having constant composition and constant specific heat. The combustion process would then be replaced by an ideal, constant pressure heat addition. Such approximations lead directly upon application of thermodynamic principles to simple formulae giving the predicted turbir3 performance for given operating conditions.

At present, the peak cycle temperatures of turbine operation are severely restricted in comparison with other types of engines due to limitations in high temperature strength of materials. For this reason the

fuel to air ratios employed in practice are maintained very lean, and consequently the assumption that working fluid composition remains constant throughout the heat addition or combustion process is relatively valid. It then appears that the simple analysis mentioned previously should be of some value in certain limited cases.

Unfortunately the simplicity of the above analysis renders it incapable of predicting performance for operation at higher temperatures and for operation with richer fuel-air mixtures. Further, it is incapable of predicting the differences in performance resulting from the use of different fuels.

Among the factors leading to deviation of real processes from those represented by the simple analysis are: the chemically reactive nature of the real working fluid and the resultant variation of fluid properties; irreversibilities occurring in the compression and expansion processes; hydrodynamic losses; and heat losses due to heat transfer from hot combustion products to surrounds.

At the temperatures prevailing following the combustion process, the normally stable products of combustion, for instance $\rm H_2^{0}$ and $\rm CO_2^{0}$, tend to dissociate forming such species as $\rm H_2^{0}$, $\rm OH_{0}^{0}$, etc. In addition, diatomic species will, to a limited extent, dissociate to form atomic species such as $\rm H_{0}^{0}$, and $\rm N_{0}^{0}$. It is thus evident that following combustion, the products of combustion retain a reactive nature which will, in principle, be exhibited throughout the expansion process with a consequent variation of

composition, and hence properties.

If it may be assumed that the time scale associated with the reactivity of combustion products is much shorter than that of the cycle processes, then the working fluid may be treated as a system always in chemical equilibrium.

According to the principles of thermodynamics, the composition and properties of any single phase reactive mixture in equilibrium are completely defined by specification of any two thermodynamic variables, for example, enthalpy, pressure, energy, etc. Chemical equilibrium conditions have beer assumed throughout this study; the details of the associated calculations are given in a later section of this report.

result generally from viscous forces associated with motion of the working fluid. The major effect is the dissipation of mechanical energy or of the kinetic energy of the working fluid by conversion to thermal energy. For purposes of analysis the effect of such dissipation is treated by defining compressor and turbine efficiencies which relate ideal, isentropic performance to the performance of real non-isentropic processes. Again the details of this treatment are left to a later part of the report.

Turning finally to the effects of hydrodynamic and heat transfer losses, it is evident that here one must consider in detail the physical design of the particular unit under consideration. Of the hydrodynamic losses, the most significant is the pressure drop sustained in the combustor. This loss is obviously highly dependent upon the combination of geometry and flow rates

employed in a particular design and cannot be treated accurately in a general analysis. Similarly, the heat loss rate will exhibit a large dependence upon the particular design and again cannot be treated in an analysis of a general nature.

While neglect of hydrodynamic and heat transfer losses will lead to predicted cycle performance deviating in absolute magnitude from that to be expected from a real engine, it is quite probable that for variations of certain parameters, for example fuel-sir ratio, the magnitudes of these losses will remain essentially constant. In this case, the ratio of theoretical performance to real performance should also remain essentially constant for all values of the parameter of interest. Hence if real engine performance is known for one value of the parameter, this ratio may be computed and applied to the entire range of values. In this way the entire real performance trend may be developed.

In this work a similar technique has been applied to the study of the influence of fuel composition on gas turbine engine performance. It was desired to predict the performance of a yet untested fuel. Identical theoretical analyses were carried out for the fuel under study and for a fuel whose real performance is well established. The performance results have been presented on a comparative basis.

Specifically, the object of this work has been the theoretical prediction of the performance of amnonia as a fuel for gas turbine-engines. The theoretical model employed is the Brayton cycle, and consideration has

been given to compressor and turbine non-idealitites and to the use of regeneration. It has been assumed that the products of combustion exist in a state of chamical equilibrium throughout the expansion process.

The effects of pressure loss through the combustor and of heat transfer to surrounds have been neglected. The reference fuel chosen is cetene (C₁₆H₃₂), a pure hydrocarbon whose composition is approximately representative of the average composition of turbine fuels currently in use. Performance results predicted for ammonia are presented relative to those predicted for cetene. Calculations involved in the analysis have been performed through use of an IBM 7094 digital computer. Thermodynamic properties of combustion products employed in this analysis are those presented in Technical Report No. 1 of this series. (1) The source of fundamental thermochemical data for this and previous work is the Joint Army-Navy-Air Force Thermo-Chemical Tables. (5)

It should be pointed out that specification of a chemical equilibrium system of combustion products implies the major assumption that ammonia can be made to burn successfully following direct injection as a liquid or vapor. While one of the major problems to be encountered in the practical development of ammonia as a turbine fuel is that of successful ignition and combustion of ammonia, the purpose of this report is the prediction of maximum potential performance to be realized.

I. THEORETICAL TECHNIQUES

1. Ideal, Non-Regenerative Brayton Cycle

The simple Brayton cycle, used as a model for the ideal gas turbine with no regeneration, is given by Figure 1 and has been described in a previous section. This cycle has been programmed for analysis using an IBM 7094 digital computer. The analytical techniques employed are described in terms of the elementary cycle processes.

a. Isentropic Compression Process

For the ideal Brayton cycle, it is assumed that compression occurs isentropically. In the computer analysis the compression process has been divided into 10 equal pressure increments determined by the given pressure ratio. Within each increment it is assumed that the charge of air undergoes isentropic compression with the isentropic exponent, $r_{\rm k}$, remaining constant throughout the increment. We then have for the k th increment,

$$P_{k+1} = P_k + \frac{P_1 \times (PR-1)}{10}$$
 (1)

$$V_{k+1} = V_k [P_k/P_{k+1}]^{1/\gamma_k}$$
 (2)

$$T_{k+1} = T_k \left[P_{k+1}/P_k\right] \frac{\gamma_k^{-1}}{\gamma_k}$$
(3)

$$H_{k+1} = M_a \qquad \int_{T_o}^{T_{k+1}} C_p (T_k) dT \qquad (4)$$

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At the end of each increment, the specific heats and isentropic exponent are adjusted according to the relationship:

$$C_{p}(T_{k}) = A + B \times T_{k} + C \times T_{k}^{2} + \dots$$
 (5)

$$C_{v}(T_{k}) = C_{p}(T_{k}) - R$$
 (6)

$$\gamma_{k} = \frac{C_{p} (T_{k})}{C_{v} (T_{k})} \tag{7}$$

where A, B, C,... are regression coefficients for the expression of specific heat as a function of temperature.

This process is repeated until state point 2 is reached at the end of the 10th increment. All pertinent working fluid properties for state point 2 have then been computed.

b. Adiabatic, Constant Pressure Combustion Process

With knowledge of the properties of the compressed charge of air at state point 2, the combustion process may be analyzed. As a direct consequence of the first law of thermodynamics, the adiabatic, constant pressure combustion process must occur with no change in total enthalpy.

Thus:

$$P_3 = P_2 \qquad (8)$$

and

$$H_3 = M_3 \sum_{j} X_j (H_{jo} + H_{js})_3 = M_2 \sum_{j} X_j (H_{jo} + H_{js})_2$$
 (9)

or since the working fluid at point 2 consists of compressed air plus liquid fuel,

$$H_{3} = M_{3} \sum_{j} X_{j} \left(H_{jo} + H_{js}\right)_{3} = M_{a} H_{a} + M_{f} \Delta H_{f}^{o} - M_{f} \Delta H_{v}^{o}$$

$$(10)$$

or

$$H_{3} = M_{3} \sum_{j} X_{j} \left(H_{jo} + H_{js}\right)_{3} = M_{s} \left[H_{s_{2}} + \left(\frac{F}{A}\right) \left(\Delta H_{f}^{o} - \Delta H_{v}^{o}\right)\right]$$
(11)

Recalling that for a chemical equilibrium system, knowledge of any two thermodynamic variables leads, in principle, to complete determination of the composition, it is seen that P_3 and H_3 are readily calculated, and hence it should be possible to find all subsequent properties.

Unfortunately, the mole fractions X_j of Equation (11) are most conveniently computed as functions of temperature and pressure which are, however, themselves dependent upon the mole fractions. For this reason it is usually necessary to resort to a trial and error technique in solving for the properties of combustion products at state point 3.

The method employed in this work provides an alternative to the usual trial and error analysis. Tachnical Report No. 1⁽¹⁾ of this series presented the composition and thermodynamic properties for combustion products of ammonia-air mixtures over a wide range of temperatures and pressures. This data has been used in conjunction with a curvilinear, least squares regression program to produce functional relationships among the various properties of combustion products pertaining to a given fuel-air mixture.

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These relations take the form of series expansions in powers of the independent variables. For example, the expression for entropy as a function of energy and volume is:

$$S = S(E, V) = A + B\sqrt{E} + C \times E + D \times E^2 + + L \ln V +$$
 (12)

where A, B, C,... are constant coefficients generated by the regression analysis as tabulated in Table 1.

For analysis of the constant pressure combustion process, the following sequence is employed.

$$P_3 = P_2 \tag{13}$$

$$H_3 = M_a \left[Ha_2 + \left(\frac{F}{A} \right) \left(\Delta H_f^0 - \Delta H_v^0 \right) \right]$$
 (14)

$$V_3 = V (H_3, P_3)$$
 (Regression equation) (15)

$$E_3 = H_3 - P_3 V_3$$
 (16)

$$S_3 = S(E_3, V_3)$$
 (Regression equation) (17)

$$T_3 = T(E_3, S_3)$$
 (Regression equation) (18)

Thus all properties of equilibrium combustion products at state point 3 may be calculated directly without resort to trial and error.

c. Isentropic Expansion Process

Following combustion, the high temperature combustion products expand isentropically to state point 4 producing useful work. For state point 4,

$$S_4 = S_3 \tag{19}$$

$$P_4 = P_1 \tag{20}$$

The usual practice in solving for the state point properties of point 4 would be the use of a trial and error technique involving adjustment of temperature and pressure. Again the regression equations described above are used to circumvent the need for a trial and error analysis and allow straightforward substitution into algebraic equations. The sequence of operations involved in solution for point 4 follows.

$$S_4 = S_3 \tag{21}$$

$$\mathbf{P}_{4} = \mathbf{P}_{1} \tag{22}$$

$$H_4 = H (S_4, P_4)$$
 (Regression equation) (23)

$$T_4 = T (S_4, P_4)$$
 (Regression equation) (24)

Following determination of properties for point 4 the performance of the cycle may be computed.

2. Non-Regenerative Cycle with Non-Ideal Compressor and Turbine

The effects of non-ideal compressor and turbine performance arise as a result of irreversibilities introduced by the existence of large gradients in the working fluid properties (i.e., temperature, pressure, velocity, etc.) in the respective flow fields. In contrast to the isentropic compression and expansion of the ideal cycle, the non-ideal processes generally exhibit

an increase in entropy. Figure 2 demonstrates this deviation, on the temperature-entropy plane, for the compression and expansion processes.

a. Non-Ideal Compressor

It is clear from Figure 2 that for a given pressure ratio, P_2/P_1 , the enthalpy ratio H_2/H_1 increases with increased entropy production, implying an accompanying increase in the required work of compression. For this reason, the compressor efficiency, η_c , is defined as:

$$\eta_{c} = \frac{H_{2}^{-H_{1}}}{H_{2}^{-H_{1}}} = \frac{T_{1} \int_{C_{p}}^{T_{2}} (T) dT}{T_{1} \int_{C_{p}}^{T_{2}} (T) dT} = \frac{Wk_{ideal}}{Wk_{real}}$$
(25)

The compressor efficiency, η_c , is a commonly used parameter and representative numerical values are readily available for various compressor types. Using a specified value of η_c , the properties corresponding to point 2' may easily be computed. The value for H_2 is first computed using Equations (1) - (7), then H_2 , is obtained from the relation:

$$H_{2} = H_{1} + (H_{2} - H_{1}) / \eta_{c}$$
 (26)

Also from (25),

$$\eta_{c} = \frac{H_{2}^{-H_{1}}}{H_{2}^{',-H_{1}}} = \frac{T_{1}}{\int_{1}^{T_{2}} C_{p}^{(T) dT}} = \frac{T_{1}}{\int_{1}^{T_{2}} C_{p}^{$$

and

$$\frac{1}{\eta_c} = 1 + \frac{T_2 \int_{-T_2}^{T_2} C_p(T) dT}{\int_{-T_2}^{T_2} C_p(T) dT} = 1 + \frac{T_2 \int_{-T_2}^{T_2} C_p(T) dT}{H_2 - H_1}$$
(28)

Now since the temperature interval $\mathbf{T_2}$ to $\mathbf{T_2}$, is much less than that from $\mathbf{T_1}$ to $\mathbf{T_2}$, that is

$$(T_2-T_1) >> (T_2, -T_2)$$

the specific heat $C_p(T)$ in the integral in (28) may be assumed substantially constant over the interval T_2 - T_2 , . Then,

$$\frac{1}{\eta_c} = 1 + \overline{C}_p \frac{(T_2, -T_2)}{H_2 - H_1}$$
 (28a)

and

as

$$T_{2'} = \frac{1}{\overline{C}_p} \left[\frac{1}{\eta_c} - 1 \right] \left[H_2 - H_1 \right] + T_2$$
 (29)

Values for T_2 and H_2 as obtained from (1) - (7) may then be substituted into (29) to obtain T_2 .

b. Non-Ideal Turbine

Referring again to Figure 2, the turbine efficiency, $\boldsymbol{\eta}_{t},$ is defined

$$\eta_{t} = \frac{H_{3}^{-H_{4'}}}{H_{3}^{-H_{4}}} = \frac{\int_{T_{4'}}^{T_{3}} C_{p}(T) dT}{\int_{T_{4}}^{T_{3}} C_{p}(T) dT}$$

hence having computed H_4 for isentropic expansion, $H_{4^{\dagger}}$ is determined from

$$H_{4'} = H_3 - \eta_t (H_3 - H_4)$$
 (31)

3. Regeneration

An increase in the thermal efficiency of the Brayton cycle may be obtained through use of regeneration. Regeneration is the use of heat from the turbine exhaust to increase the temperature of the compressed air charge prior to combustion. In this way it is possible to utilize a portion of the exhaust heat which would otherwise produce no useful work if rejected to surrounds.

The Brayton cycle as modified by addition of a regenerator is shown in Figure 3. The regenerator is here shown as a counterflow heat exchanger and the temperature of the high-pressure gas leaving the regenerator, T_5 , may, in the ideal case, be equal to T_4 , temperature of the gas leaving the turbine.

The exchange of heat between exhaust initially at point 4' and compressed air charge at 2' results in an increase in enthalpy of the compressed charge to point 5. The enthalpy at point 5, H₅, is determined by the regenerator

effectiveness, $\epsilon_{\mathbf{r}}$, which is given by

$$\epsilon_{\mathbf{r}} = \frac{H_{5}^{-H_{2'}}}{H_{4'}^{-H_{2'}}} = \frac{\int_{\mathbf{T}_{2'}}^{\mathbf{T}_{5}} C_{\mathbf{p}}(\mathbf{T}) d\mathbf{T}}{\int_{\mathbf{T}_{2'}}^{\mathbf{T}_{4'}} C_{\mathbf{p}}(\mathbf{T}) d\mathbf{T}}$$
(32)

then,

$$H_5 = \epsilon_r (H_4, - H_2,) + H_2,$$

Since H_4 , is dependent upon the value of H_5 which is not known a priori, an iterative technique must be used in solution of the regenerative Brayton cycle. As a first approximation, the compression process is carried out and an estimated value for H_5 is used in completing solution of combustion and expansion processes. The value of H_4 , so obtained is then inserted in (32) to determine a more accurate estimate of H_5 for a second cycle calculation. The values for H_4 , resulting from the first and second cycle calculations are then compared and if agreement is not satisfactory, the process is repeated. Convergence is indicated by agreement of values for H_4 , of no greater than 1% deviation for two consecutive iterations.

4. Cycle Performance

Following complete determination of working fluid properties at each point of the theoretical cycle the corresponding cycle performance may be calculated.

a) Work Output

The work output produced by an engine operating on the Brayton cycle, as given by Figures 1, 2 or 3, is the work produced by the turbine less that amount required in compression of the fresh charge of air.

From the first law of thermodynamics, the work done by a steady flow compressor operating between points 1 and 2' is given by,

$$Wk_{com} = (H_2, - H_1)$$

Similarly for a turbine operating between points 3 and 4',

$$Wk_{turb} = (H_3 - H_4)$$

hence,

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$$Wk_{net} = (H_3 - H_4') - (H_2' - H_1)$$
 (33)

b) Thermal Efficiency

The thermal efficiency, defined as the ratio of useful work output to the fuel energy supplied is given by,

$$\eta_{th} = \frac{W_{net}}{(LHV)_{f} \times W_{f}}$$
 (34)

c) Specific Fuel Consumption

The specific fuel consumption, a practical indication of the operational aconomy of a cycle, is defined as the weight of fuel required to produce

one horse-power for one hour.

$$SFC = \frac{W_f}{Wk_{net}} \times 2545 \tag{35}$$

II. THEORETICAL RESULTS

1. Influence of Peak Cycle Temperatures

In the operation of gas turbines of the type currently in general use, one of the most critical operating parameters is the turbine inlet temperature. This corresponds to the peak cycle temperature of the associated Brayton cycle. Thus, the power output obtainable from a given turbine is determined by the fuel-to-air ratio which is limited by this maximum permissible turbine inlet temperature. From the standpoint of maximum power output, the most desirable fuel is one which will produce the greatest quantity of work for a given peak cycle temperature.

Among the factors which determine the peak temperature resulting from combustion of a given fuel are the energy content or heating value of the fuel, the latent heat of vaporization of the fuel and the total heat capacity of products resulting from combustion of the fuel. The heat capacity of products is dependent not only upon the heat capacities and concentrations of individual species present, but also upon the total number of moles of product produced and upon the degree of dissociation. Generally, excluding dissociation effects, a fuel favoring the generation of relatively low combustion temperatures would be one having a low energy content, a high latent heat of vaporization and one which produces a relatively large number of moles of products.

Comparing ammonia with the hydrocarbon fuels, one finds that ammonia exhibits a slightly higher energy content, a much higher latent heat of vaporization, and in addition, the number of moles of products produced by ammonia is significantly greater than that produced by hydrocarbon fuels.

On this basis one would expect that, as substantiated by Figures 4-7, peak cycle temperatures produced by ammonia should be comparatively much less than those produced by hydrocarbon fuels.

Figure 4 shows the peak cycle temperatures obtainable as a function of fuel-air equivalence ratio for the non-regenerative Brayton cycle. Compressor and turbine isentropic efficiencies have no significant influence on peak temperatures, and the results presented apply equally well for all such efficiencies in the range 0.85-1.0. As indicated by Figure 4, temperatures produced by ammonia at any given percent of stoichiometric mixture are significantly lower than those produced by hydrocarbon fuels. This temperature difference, amounting to some 600°R at the chemically correct mixture ratio, decreases continuously with decreasing fuel to air ratio. Obviously the temperatures for both ammonia and hydrocarbon fuels converge to the compression temperature in the limit as fuel-air ratio approaches zero.

The influence of cycle pressure ratio upon peak cycle temperature for the non-regenerative Brayton cycle is shown in Figure 5. These curves also apply to cycles with compressor and turbine isentropic efficiencies ranging from 0.85 to 1.0. Peak cycle temperature is only moderately dependent upon pressure ratio in contrast to the high degree of dependence

upon the fuel-air ratio. Further it is noted that for a given fuel-air ratio the difference in temperature between ammonia combustion and hydrocarbon combustion remains nearly constant over the entire range of pressure ratios considered, and hence this temperature difference is dependent primarily upon fuel-air ratio.

Figures 6 and 7 present peak cycle temperatures for the regenerative Brayton cycle. In the regeneration process energy recovered from the exhaust in addition to the energy of the fuel is supplied to the fresh charge. As a consequence, peak cycle temperatures for a given fuel-air ratio are substantially increased by regeneration, as indicated by Figures 6 and 7.

The influence of fuel-air ratio upon peak cycle temperature for the regenerative Brayton cycle is shown in Figure 6. While temperatures are generally higher than for the non-regenerative cycle, it is again apparent that at any given equivalence ratio ammonia yields lower peak cycle temperatures than hydrocarbon fuels. For the regenerative cycle the difference between ammonia and hydrocarbon peak cycle temperatures for a constant fuel-air ratio also increases with increasing fuel-to-air ratio.

With the use of regeneration, the peak cycle temperature is influenced not only by fuel properties, but also by the temperature of exhaust products following expansion. In general, an increase in cycle pressure ratio will result in an increase in compression temperature and a decrease in the difference between compression and exhaust temperatures with the latter effect reducing the energy transfer in the regenerator. Thus the peak cycle

the influence of cycle pressure ratio upon peak cycle temperature. For the leaner fuel-air ratios one observes a critical pressure ratio at which the peak cycle temperature is a minimum. Below the critical pressure ratio, the temperature difference between compression and exhaust dominates; however, for higher pressure ratios the effect of increasing compression temperature is dominant. In all cases it is seen that ammonia temperatures are less than hydrocarbon temperatures.

2. Power Output

The power output to be obtained from a Brayton cycle engine operating with a given cycle pressure ratio and a given fuel-air ratio is governed largely by the energy content of the fuel, by the number of product moles resulting from combustion of that fuel and by the latent heat of vaporization of the fuel. For most conventional heat engines, power output is determined or controlled by the fuel-air ratio. Maximum output occurs in the vicinity of the chemically correct ratio. Unfortunately, in the case of presently available gas turbines, fuel-air ratios are limited to very lean values due to the limitation of turbine inlet temperatures. For this reason, gas turbine operation is characterized by control of turbine inlet temperature rather than fuel-air ratio. Accordingly, further results of this study are presented with turbine inlet temperature rather than fuel-air ratio as controlling parameter.

Figure 8 presents power output for the non-regenerative ideal Brayton cycle as influenced by turbine inlet temperature. It indicates that the combined effects of high heat of vaporization and high yield of product moles for ammonia tend to yield increasingly superior performance for ammonia over cetene as the temperature increases. According to Figure 8, the power produced by ammonia converges to that of cetene for temperatures less than 2000° R, a result of the diminishing quant less of fuel present. On the other hand, at temperatures in the vicinity of 4000° R, the predicted power output of ammonia exceeds that for cetene by 20%.

The influence of cycle pressure ratio on ideal, non-regenerative

Brayton cycle power is given by Figure 9 for several turbine inlet temperatures

It is evident that for a given temperature, the difference in performance

between that of ammonia and that of cetene is only moderately influenced by

pressure ratio.

Figure 10 presents normalized ideal Brayton cycle power relative to that produced by hydrocarbon fuels operating at a turbine inlet temperature of 2000°R. The increasing superiority of performance with increasing turbine inlet temperature of ammonia over hydrocarbon fuels is clearly demonstrated. as is the almost insignificant effect of cycle pressure ratio upon relative performance.

The predicted power output for non-ideal, non-regenerative Brayton cycles having compressor and turbine isentropic efficiencies of 0.85 is presented in Figures 11, 12, and 13. It is apparent that compressor and

Figure 14 presents power output for the regenerative Brayton cycle as influenced by turbine inlet temperature. Again it is noted that for a given temperature and pressure ratio, ammonia produces greater power output than does the hydrocarbon fuel.

Power output for the regenerative cycle as influenced by pressure ratio is shown in Figure 15. The beneficial effects of regeneration depend upon the difference between exhaust temperature and compression temperature. As this temperature difference decreases, due to increasing pressure ratio, the effect of regeneration diminishes resulting in the existence of an optimum pressure ratio yielding maximum output. As peak cycle temperature increases, the optimum pressure ratio for maximum output shifts toward increasing values of pressure ratio.

3. Thermal Efficiency

Thermal efficiency, a measure of the degree of utilization of fuel energy, is determined mainly by controlled engine operating parameters of which cycle pressure ratio and turbine inlet temperature are the most important.

To a lesser extent, thermal efficiency is influenced by the thermodynamic properties of combustion products, of which, as previously discussed, the yield of product moles is one of the most important. In general, for given

operating conditions, high thermal efficiencies are favored by fuels producing a large yield of product moles. In view of the substantial number of product moles obtained from ammonia as contrasted to hydrocarbons, ammonia would be expected to yield thermal efficiencies greater than those of hydrocarbon fuels.

Figures 16 and 17 present predicted thermal efficiencies for non-regenerative Brayton cycle engines. It is evident that ammonia exhibits higher thermal efficiencies than hydrocarbon fuels as anticipated from the analysis of product moles produced.

Figures 18 presents the influence of turbine inlet temperature on regenerative Brayton cycle thermal efficiency. Again, the thermal efficiency for ammonia is substantially greater than that for hydrocarbon fuels for equal turbine inlet temperatures. Regenerative cycle thermal efficiency as influenced by cycle pressure ratio is given by Figures 19.

4. Specific Fuel Consumption

In the practical evaluation of the efficiency of engine operation, specific fuel consumption is often of more significance than thermal efficiency. Specific fuel consumption is defined as the weight of fuel consumed per unit work output produced.

Figures 20 and 21 present predicted specific fuel consumption for the non-regenerative Brayton cycle. Even though ammonia exhibits a higher predicted thermal efficiency than do hydrocarbon fuels, the abundance of the inert constituent, nitrogen, requires a relatively large weight of ammonia to be burned for a given energy release which results in high values

of specific fuel consumption. The predicted specific fuel consumption for ammonia is approximately 2-1/2 times that of the hydrocarbon fuel over the entire range of operation for the non-regenerative cycle.

Specific fuel consumption for the regenerative cycle is shown in Figures 22 and 23. For given turbine inlet temperature and pressure ratio, specific fuel consumption for ammonia ranges from 2-1/2 to 3 times that for hydrocarbon fuels over the entire range of operation for the regenerative cycle.

The variation of fuel consumption with pressure ratio in Figures 21 and 23 indicates minimum values of specific fuel consumption corresponding to maximum values of thermal efficiency in Figures 17 and 19.

Figures 24 through 39 of the Appendix are representations of performance as defined by certain other parametric relationships than those presented in the body of the report. Principally, the parameter of peak cycle temperature has not been considered as a limiting variable in most of these curves. They would therefore relate to operation of a cycle for which turbine material was generally not a limiting factor.

CONCLUSIONS

- 1) In the event of developments leading to successful combustion of ammonia in gas turbine applications, ammonia would be expected to yield power output up to 10% greater than that for hydrocarbon fuels operating under the same conditions.
- 2) Thermal efficiencies for ammonia should range up to 10% higher than those for hydrocarbon fuels operating at the same conditions.
- 3) Specific fuel consumption for ammonia would be expected to range from2-1/2 to 3 times that for hydrocarbon fuels.

MATHEMATICAL SYMBOLS

Wk

work, Btu/lb-air

temperature, OR pressure, psia volume, ft3/lb-air enthalpy, Btu/lb-air H enthalpy of formation of species j, Btu/mole Hot sensible enthalpy of species j, Btu/mole Hjs enthalpy of 1 lb of air H specific heat at constant pressure, Btu/mole-OR specific heat at constant volume, Btu/mole-OR specific heats ratio, C_p/C_v Υ M moles M moles of air/lb-air mole fraction of species j heat of formation at standard conditions, Btu/mole ∆H^o heat of vaporization at standard conditions, Btu/mole fuel-air ratio, molar F/A entropy, Btu/lb-air-OR S E internal energy, Btu/lb-air- $\eta_{\mathbf{c}}$ compressor isentropic efficiency turbine isentropic efficiency $\boldsymbol{\eta_t}$

 ϵ_{r} regenerator effectiveness

 η_{th} thermal efficiency

(LHV) lower heat value of fuel, Btu/lb

SFC specific fuel consumption, lbs/hp-hr

PR cycle pressure ratio

W weight of fuel supplied, lks per cycle

X

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- 1) H. K. Newhall, "Chemical Equilibrium Properties of Ammonia-Air Combustion Products", Technical Report No. 1 under contract DA-04-200-AMC-791(x) Ammonia Fuel, Army Material Command, R & D Directorate, 1964.
- 2) H. K. Newhall, "Calculation of Engine Performance Using Ammonia Fuel,

 I. Otto Cycle", Technical Report No. 2 under contract DA-04-200-AMC-791(x),

 Ammonia Fuel, Army Material Command, R & D Directorate, 1965.
- 3) H. K. Newhall, "Calculation of Engine Performance using Ammonia Fuel, II. Diesel Cycle", Technical Report No. 3, Under contract DA-04-200-AMC-791(x) Ammonia Fuel, Army Material Command, R & D Directorate, 1965.
- 4) "JANAF Interim Thermochemical Data Tables", by The Joint Army-Navy-Air Force Thermochemical Panel. ARPA Program USAF Contract
 AF33(616)-6149, Thermal Laboratory, Dow Chemical Corp., Midland,
 Michigan, December 1960.

Table 1. Regression Coefficients for Entropy as A Function of Energy and Volume for Ammonia-Air Combustion Products

 $S=A+B\sqrt{E^*}+CxE^*+DxE^*+FxE^*+GxE^*+Hx\ln V+Ix(\ln V)^2+Jx(\ln V)^3+Kx(\ln V)^4+Lx(\ln V)^5$

<u>Where</u>: $\vec{E}^* = E+2000.0$ -Btu, $V = Volume-Ft.^3$, $S = Entropy-Btu/^OR:-lb-air$

Equivalenc Ratio	e A	В	С	D		F
0.2	-3.020	1.211x10	-1 o	0	-6.9	990x10 ⁻⁵
0.4	3.256x10	-3 5.159x10	-2 0	-6.336	x10 ⁻⁴	0
0.6	8.947x10			0		0
0.8	9.656x10		-2 0	-4.853	x10 ⁻⁴	0
1.0	1.412	3.448x10	-2 -1,866x	0		0
Equivalenc	:e	· · · · · · · · · · · · · · · · · · ·				
Ratio	G	H	I	J	K	L
0.2	0		-1.673x10 ⁻⁵	0	0	0
0.4	0	7.843×10^{-2}	0	0	0	-5.408x10
0.6	-2.229x10 ⁻⁷	8.092x10 ⁻²	1.864x10 ⁻³	0	-9.637x10	-4 2.669x10
0.8	0	8.771x10 ⁻²	2.068x10 ⁻³	$-1.507x10^{-3}$	2.568x10	-4 0
1.0	0	9.044×10^{-2}	$-2.673x10^{-4}$	0	0	0

Table 2. Regression Coefficients for Temperature As A Function of Energy and Entropy for Ammonia-Air Combustion Products

T=A+Bx\(\overline{E}\)\(\text{

quivalenc	e					
Ratio	Α	В	С	D	F	G
0.2	-19,060	487.6	0	0	-9.298x10 ⁻²	0
0.4	-12,510	355.1	0	0	0	0
0.6	- 9,606	311.5	0	0.1259	0	0
0.8	- 6,908	262.6	0	0.9028	0	0
1.0	- 5,425	247.4	0	0	0	2.079x10 ⁻³

Equivalence								
Ratio	Н	I	J	K	L	M		
0.2	0	o	0	0	0	0		
0.4	1.018x10 ⁻⁵	0	0	-2.069×10^{-2}	0	0		
0.6	0	0	-0.5929	0	0	0		
0.8	0	0	-0.7533	0	0	0		
1.0	0	7.692	-1.399	0	0	0		

Table 3. Regression Coefficients for Volume As A Function of Enthalpy and Pressure for Ammonia-Air Combustion Products $V=A+B\times(\frac{H}{P}^{*})+C\times(\frac{H}{P}^{*})^{2}+D\times(\frac{H}{P}^{*})^{3}+F\times(\frac{H}{P}^{*})^{4}+G\times(\frac{H}{P}^{*})^{5}$

V = Volume-Ft³/lb-air, H = H+2000. = Enthalpy-Btu/lb-air, P = Pressure-psia

Equivalence Ratio	A	В	С	D	F	G
0.2	-1.161	0.4838	0	0	-9.763×10^{-6}	2.025x10 ⁻⁷
0.4	-0.9229	0.5735	0	0	-1.089×10^{-5}	
0.6	-0.4409	0.7283	0	0	-3.409×10^{-6}	7.582x10 ⁻⁸
0.8	-0.5895	1.002	-9.036x10 ⁻³	1.062x10	0	1.179x10 ⁻⁸
1.0	-0.0155	1.000	0	0	0	-2.191×10^{-9}

Table 4. Regression Coefficients for Temperature As A Function of Entropy At Atmospheric Pressure for Ammonia-Air Combustion Products

 $T=A+BxS+CxS^{2}+DxS^{3}+ExS^{4}+FxS^{5}$ $T = Temperature - {}^{O}R, S = Entropy - Btu/{}^{O}R-lb-air$

ivalence		_			_	To
Ratio	A	<u>B</u>	c	D	E	<u> </u>
0.2	3838	-2719	0	0	0	90.05
0.4	352 3	-2362	0	0	0	64.16
0.6	3068	-1985	0	0	0	47.82
0.8	987.5	0	-438.7	0	0	37.88
1.0	2537	-1503	0	0	0	26.80

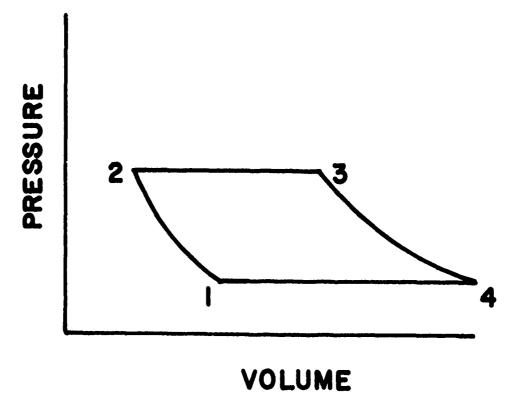
Table 5. Regression Coefficients for Enthalpy As A Function of Entropy at Atmospheric Pressure for Ammonia-Air Combustion Products

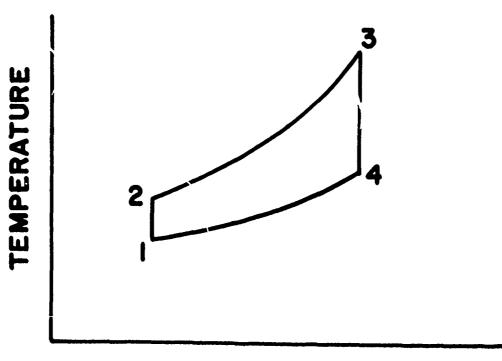
 $H=A+BxS+CxS^2+DxS^3+FxS^4+GxS^5$

H = Enthalpy - Btu/lb-air, S = Entropy - Btu/lb-air-OR

uivalence									
Ratio	<u>A</u>	В	<u> </u>	D	F	G			
0.2	563	O	-466.7	0	0	38.79			
0.4	295	0	-430.6	0	0	30.09			
0.6	0	0	-394.2	0	0	24.18			
0.8	-311	0	-355.8	0	0	19.09			
1.0	-578	0	-333.9	0	0	15.55			

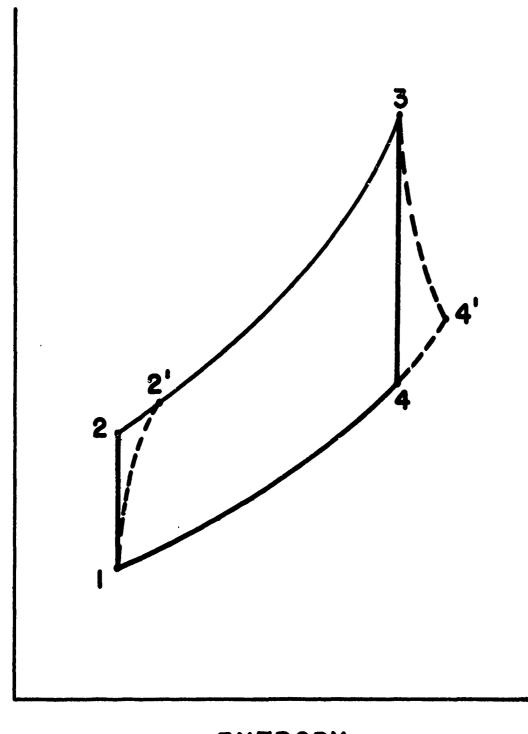






ENTROPY

BRAYTON GYCLE WITH NON-IDEAL COMPRESSION AND EXPANSION



TEMPERATURE

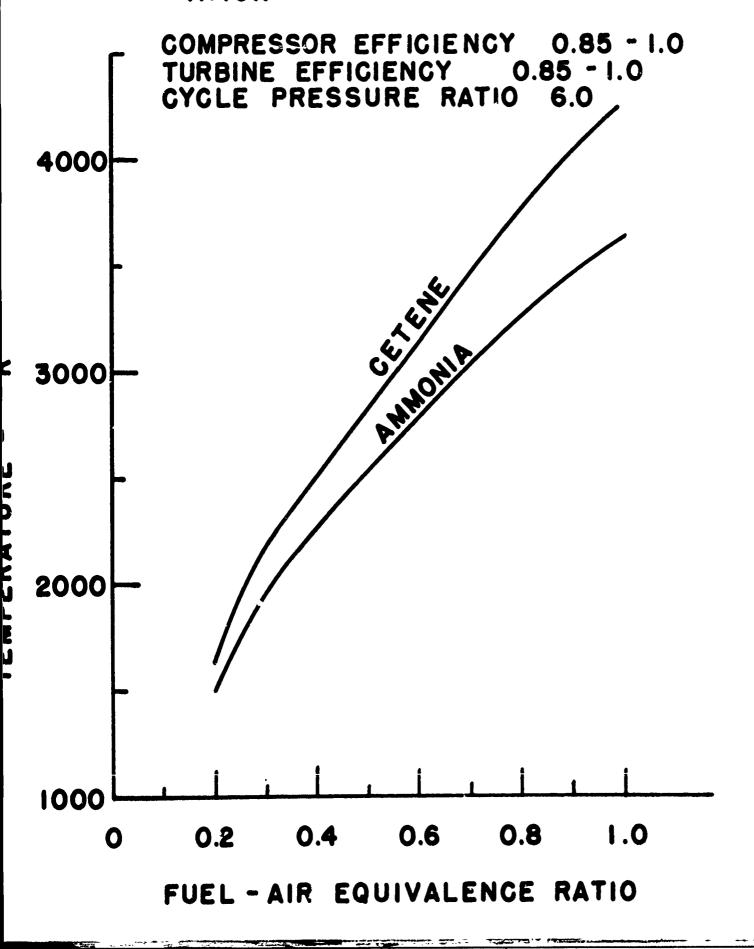
ENTROPY

TEMPERATURE

ENTROPY

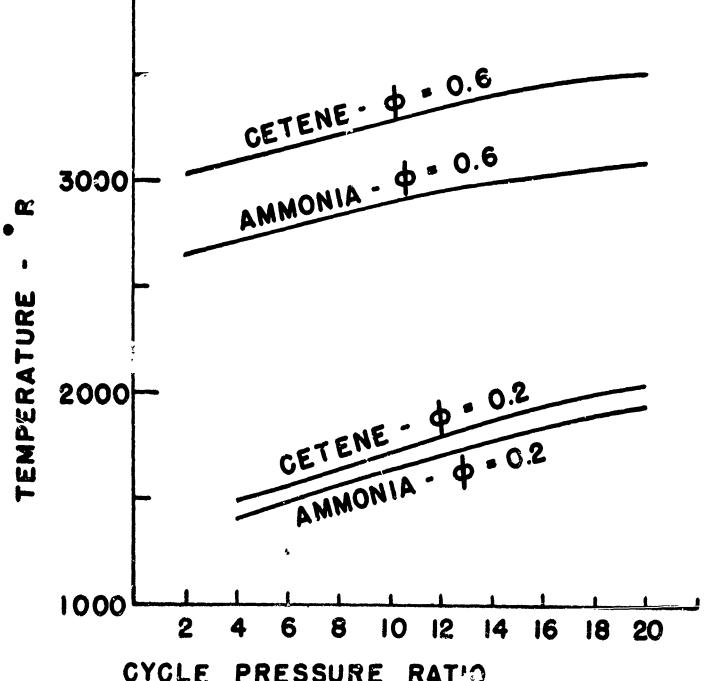
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INFLUENCE OF FUEL-AIR RATIO UPON
THEORETICAL PEAK CYCLE TEMPERATURE
FOR BRAYTON CYCLE WITH NO REGENERATION



INFLUENCE OF PRESSURE RATIO ON PEAK CYCLE TEMPERATURE FOR BRAYTON CYCLE WITH NO REGENERATION

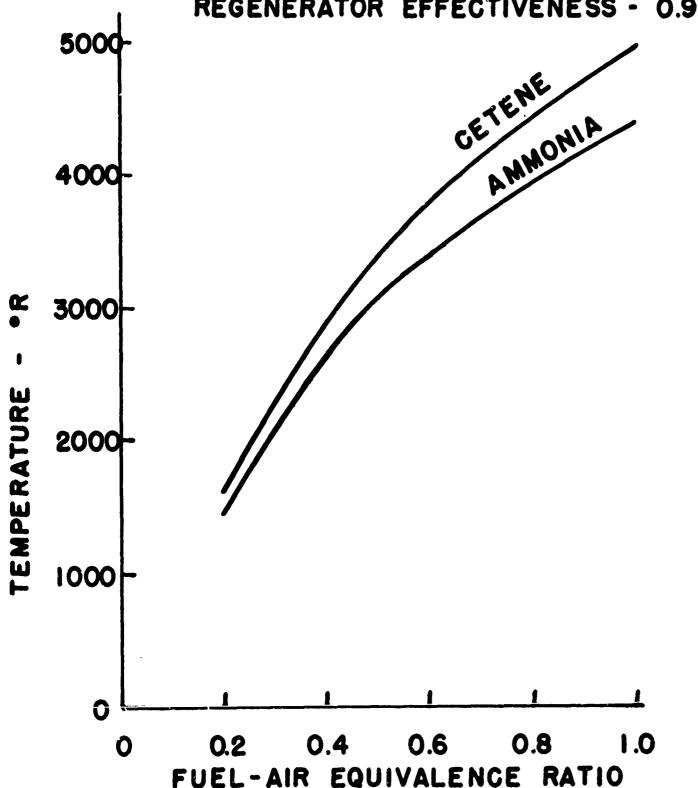
φ = FUEL-AIR EQUIVALENCE RATIO COMPRESSOR EFFICIENCY 0.85 - 1.0TURBINE EFFICIENCY 0.85 - 1.04000



CYCLE PRESSURE RATIO

INFLUENCE OF FUEL-AIR RATIO UPON PEAK TEMPERATURE FOR THEORETICAL REGENERATIVE BRAYTON CYCLE

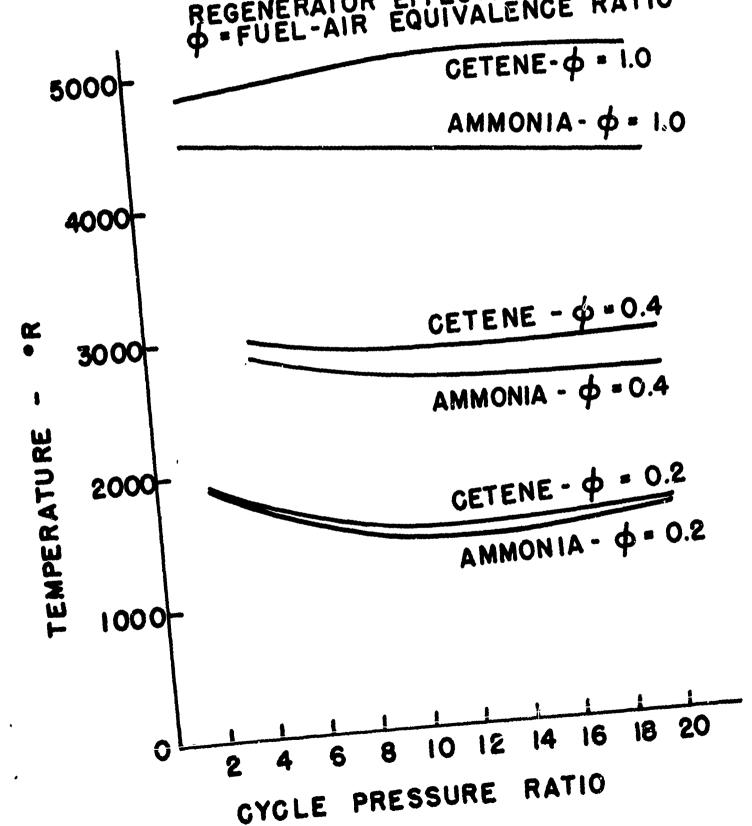
CYCLE PRESSURE RATIO - 8:1 COMPRESSOR EFFICIENCY - 0.85 TURBINE EFFICIENCY - 0.85 REGENERATOR EFFECTIVENESS - 0.9



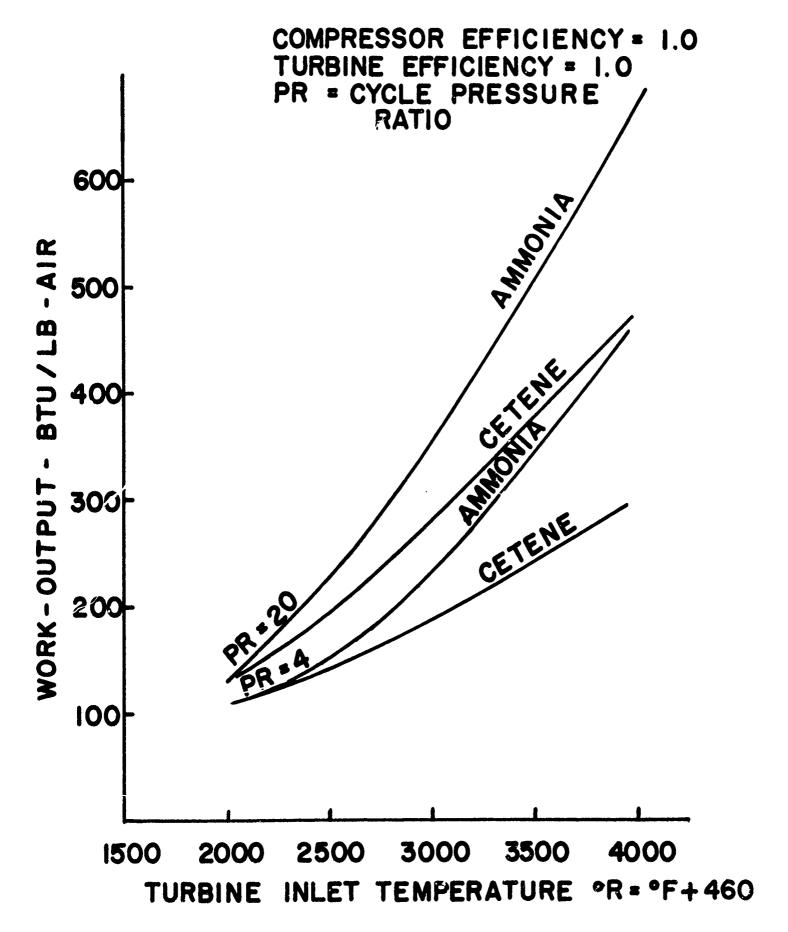
PEAK TEMPERATURE AS INFLUENCED BY CYCLE PRESSURE RATIO FOR THEORETICAL REGENERATIVE BRAYTON CYCLE

COMPRESSOR EFFICIENCY - 0.85
TURBINE EFFICIENCY - 0.85
REGENERATOR EFFECTIVENESS - 0.90
REGENERATOR EQUIVALENCE RATIO

FUEL-AIR EQUIVALENCE RATIO

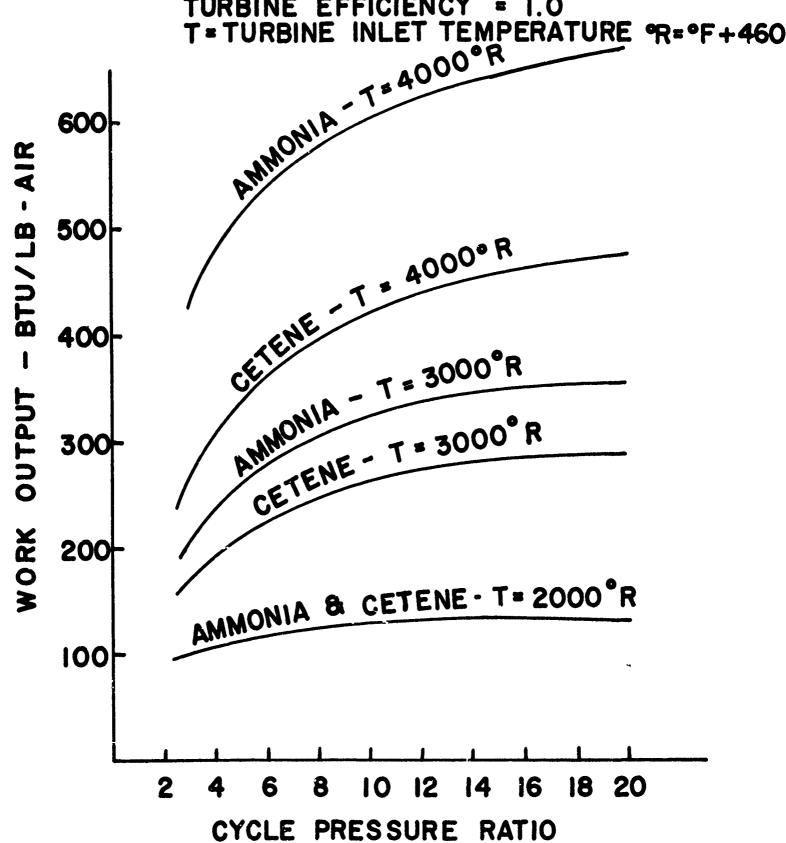


VARIATION OF THEORETICAL BRAYTON CYCLE POWER OUTPUT WITH TURBINE INLEY TEMPERATURE - NO REGENERATION



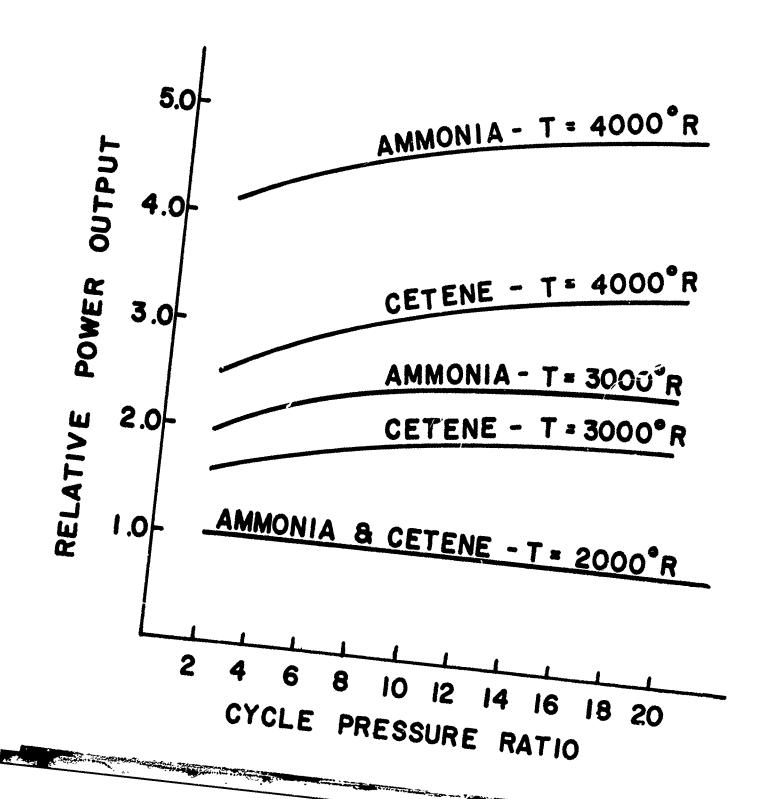
INFLUENCE OF CYCLE PRESSURE RATIO UPON POWER OUTPUT OF THEORETICAL BRAYTON REGENERATION

> COMPRESSOR EFFICIENCY = 1.0 TURBINE EFFICIENCY TEMPERATURE %= °F+460



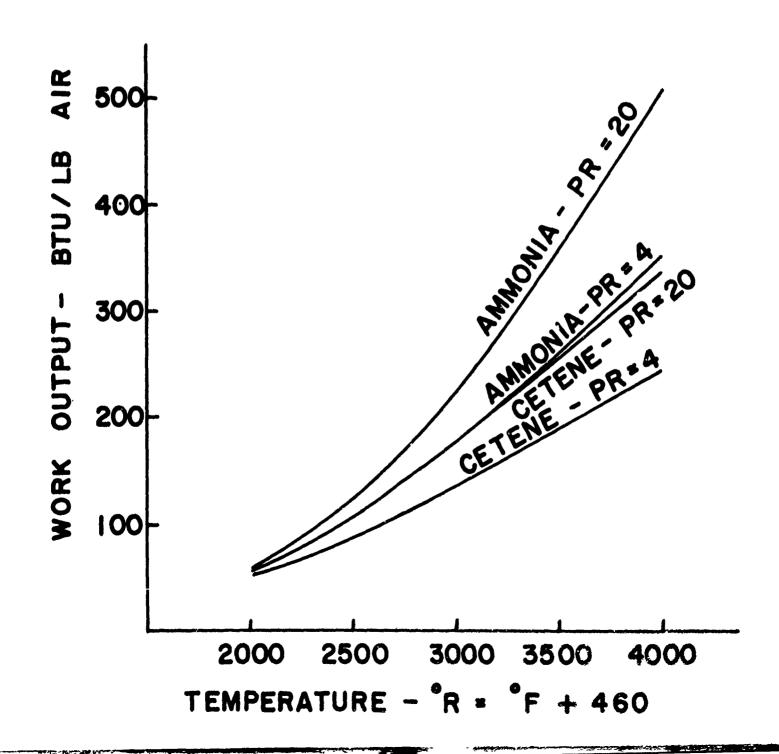
NORMALIZED POWER OUTPUT FOR THEORETICAL BRAYTON CYCLE WITH NO REGENERATION

COMPRESSOR EFFICIENCY = 1.0
TURBINE EFFICIENCY = 1.0
T = TURBINE INLET TEMPERATURE*R = *F + 460



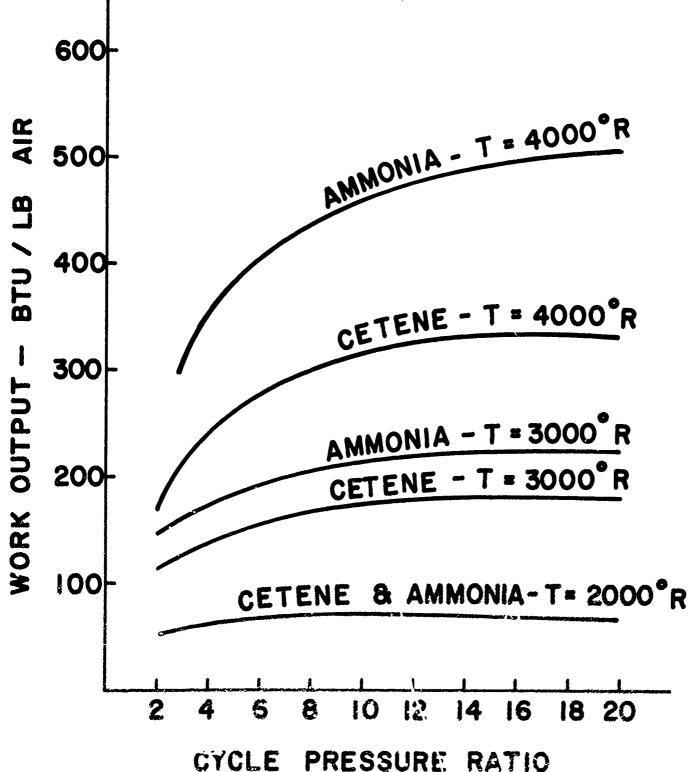
VARIATION OF THEORETICAL BRAYTON CYCLE POWER OUTPUT WITH TURBINE INLET TEMPERATURE - NO REGENERATION

COMPRESSOR EFFICIENCY = 0.85 TURBINE EFFICIENCY = 0.85



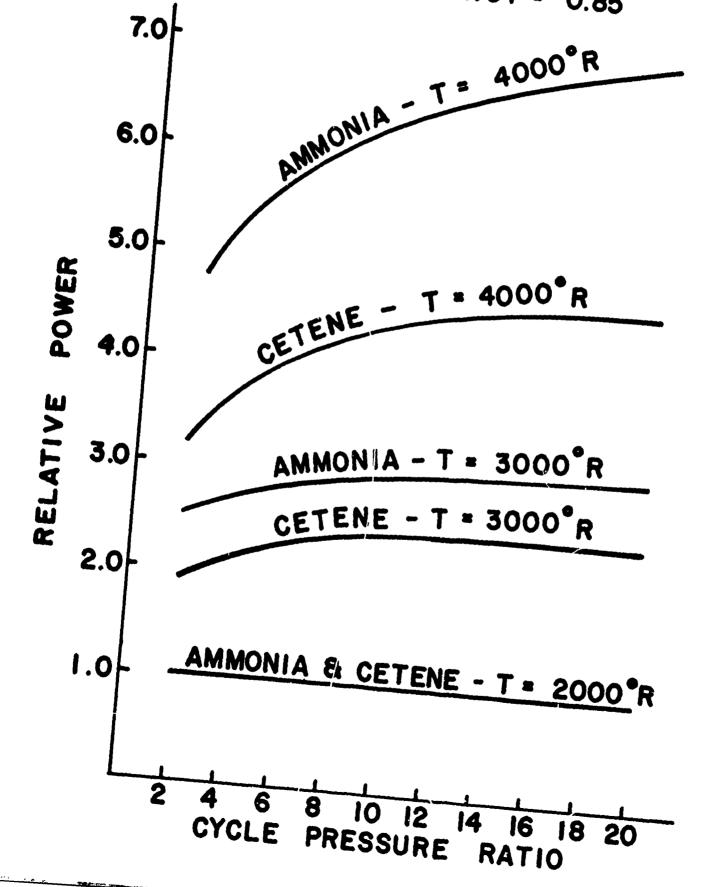
INFLUENCE OF CYCLE PRESSURE RATIO UPON POWER OUTPUT OF THEORETICAL BRAYTON CYCLE WITH NO REGENERATION

COMPRESSOR EFFICIENCY = 0.85 TURBINE EFFICIENCY = 0.85 T = TURBINE INLET TEMPERATURE -R = F + 460



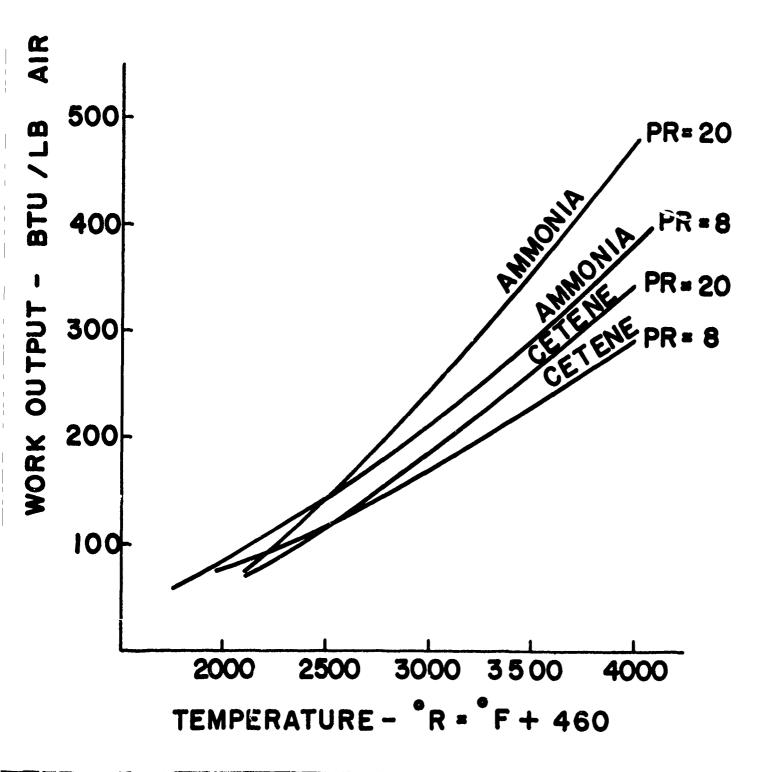
NORMALIZED POWER OUTPUT FOR THEORETICAL BRAYTON CYCLE WITH NO REGENERATION

COMPRESSOR EFFICIENCY = 0.85 TURBINE EFFICIENCY = 0.85



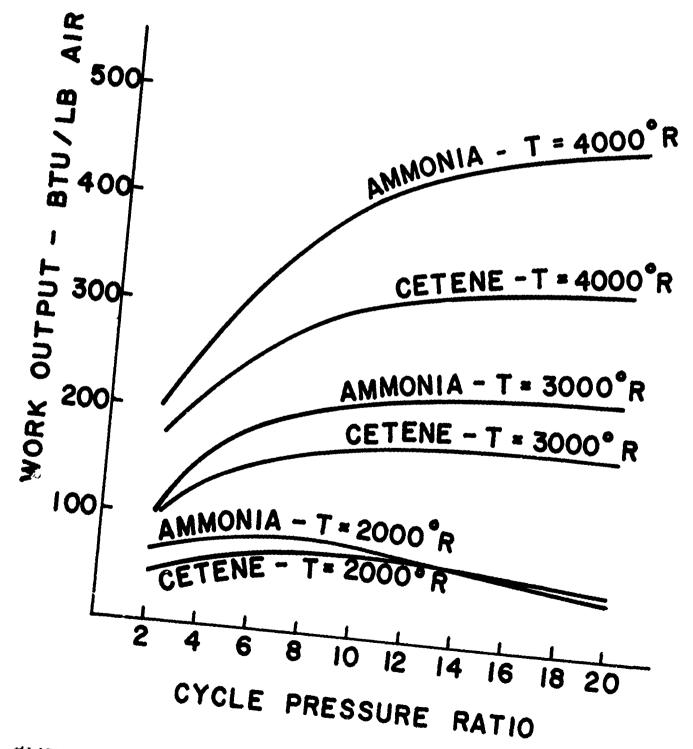
VARIATION OF THEORETICAL REGENERATIVE BRAYTON CYCLE POWER OUTPUT WITH TURBINE INLET TEMPERATURE

COMPRESSOR EFFICIENCY = 0.85 TURBINE EFFICIENCY = 0.85 REGENERATOR EFFECTIVENESS = 0.9 PR = CYCLE PRESSURE RATIO



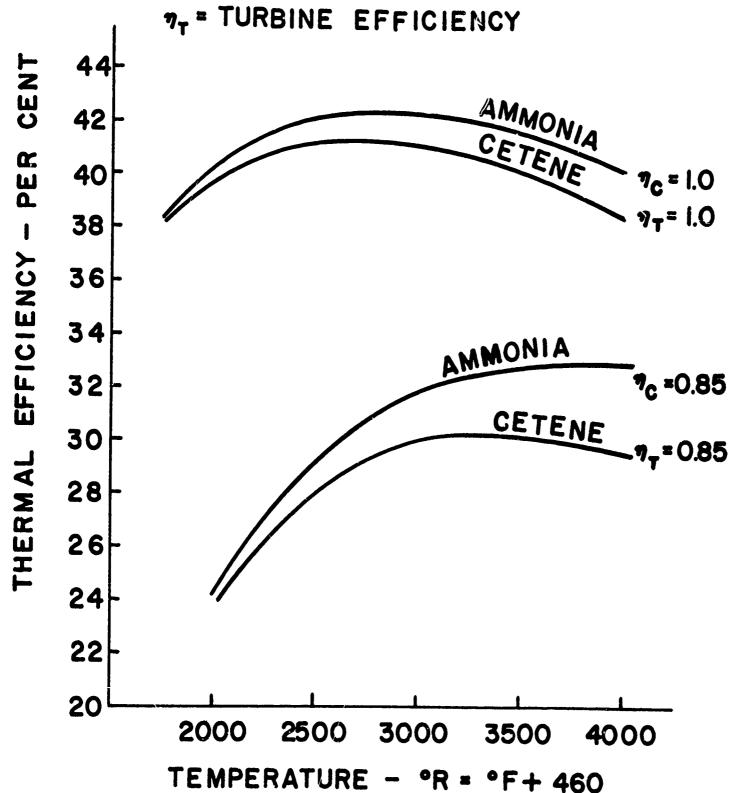
INFLUENCE OF PRESSURE RATIO UPON POWER OUTPUT FOR REGENERATIVE BRAYTON CYCLE

COMPRESSOR EFFICIENCY = 0.85
TURBINE EFFICIENCY = 0.85
REGENERATOR EFFECTIVENESS = 0.9
T = TURBINE INLET TEMPERATURE R = F + 460

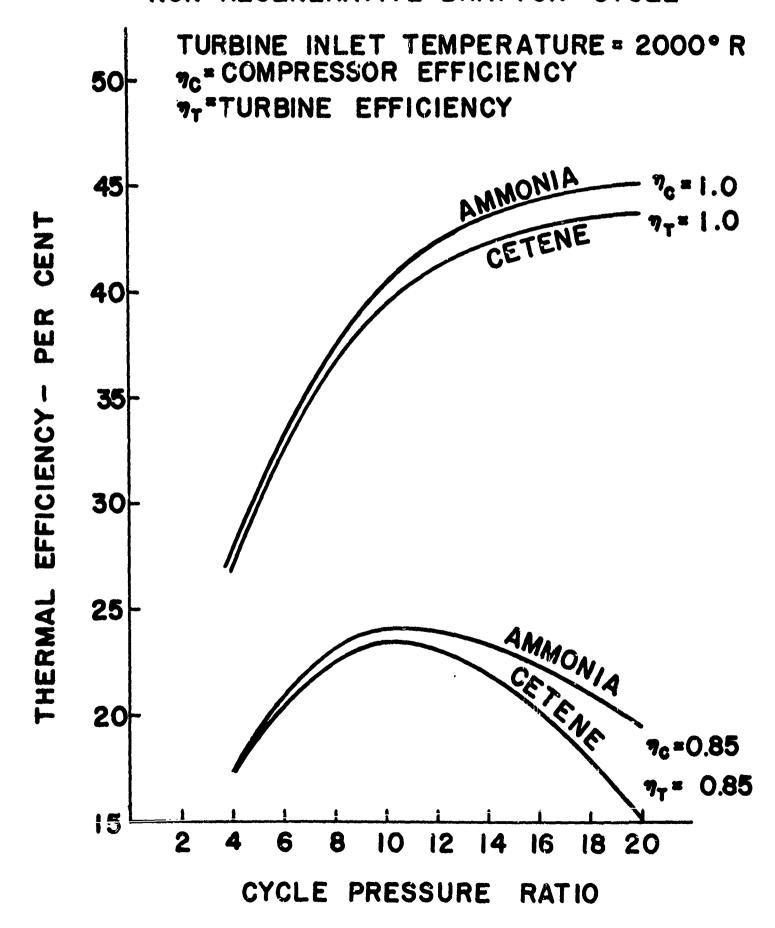


VARIATION OF THERMAL EFFICIENCY OF THEORETICAL NON-REGENERATIVE BRAYTON CYCLE WITH TURBINE INLET TEMPERATURE

CYCLE PRESSURE RATIO = 10.0 7c = COMPRESSOR EFFICIENCY 7T = TURBINE EFFICIENCY

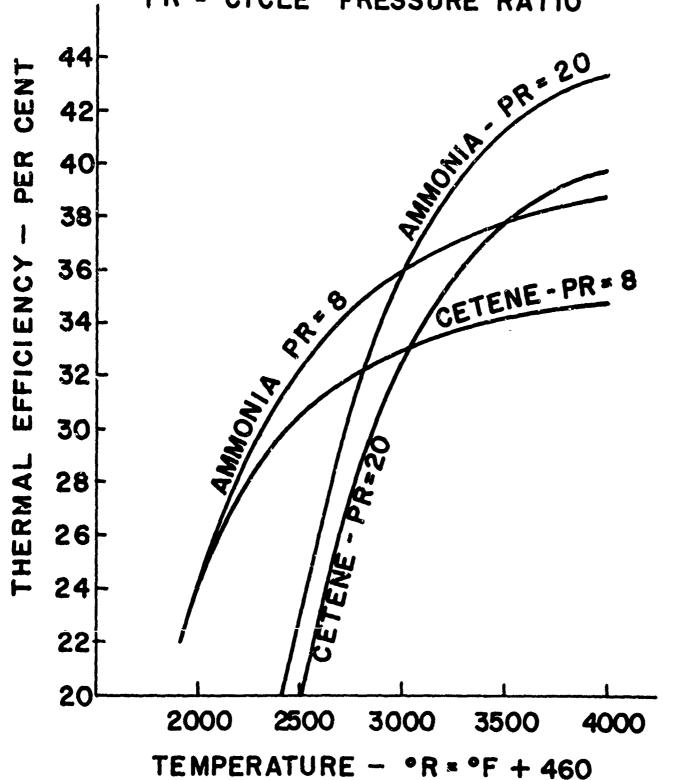


INFLUENCE OF CYCLE PRESSURE RATIO UPON THERMAL EFFICIENCY OF THEORETICAL NON-REGENERATIVE BRAYTON CYCLE



INFLUENCE OF TURBINE INLET TEMPERATURE UPON THERMAL EFFICIENCY OF THEORETICAL REGENERATIVE BRAYTON CYCLE

COMPRESSOR EFFICIENCY = 0.85 TURBINE EFFICIENCY = 0.85 REGENERATOR EFFECTIVENESS = 0.9 PR = CYCLE PRESSURE RATIO



INFLUENCE OF CYCLE PRESSURE RATIO ON THERMAL EFFICIENCY OF THEORETICAL REGENERATIVE BRAYTON CYCLE

EFFICIENCY = 0.85 COMPRESSOR TURBINE **EFFICIENCY** REGENERATOR EFFECTIVENESS = T = TURBINE INLET TEMPERATURE = °F + 460 50 AMMONIA-T = 4000 ° R CETENE - T= 4000 °R 40 AMMONIA - T= 3000°R CETENE - T = 3000 °R THERMAL EFFICIENCY 30 AMMONIA 20 10 0 2 6 8 10 12 14 16 18 20 CYCLE **PRESSURE** RATIO

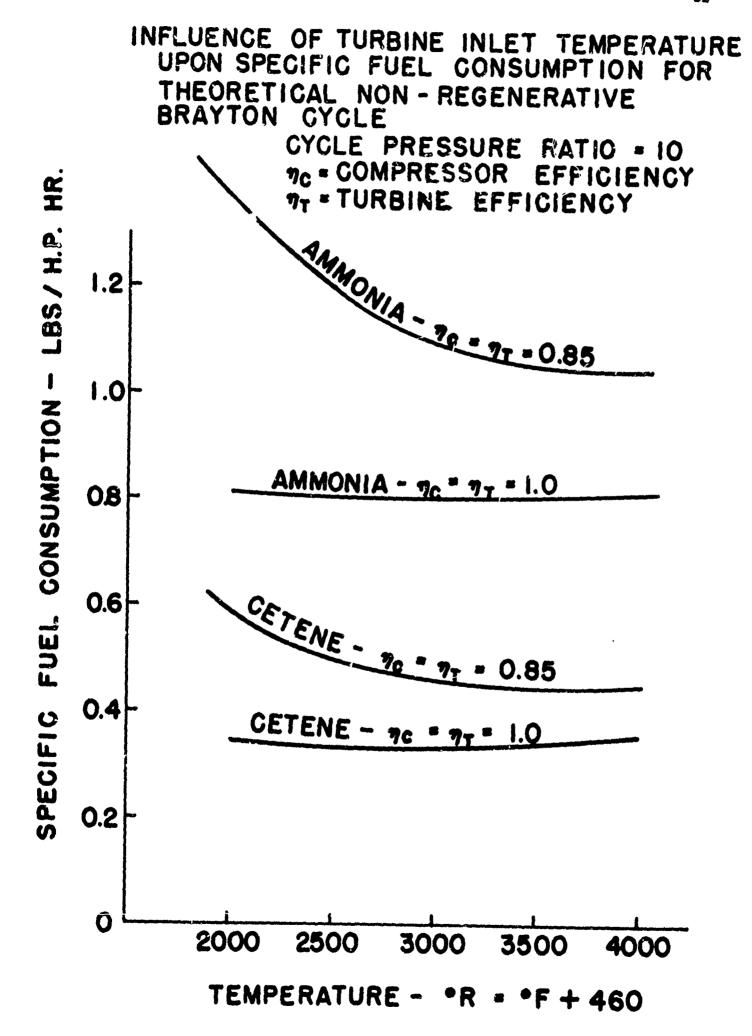
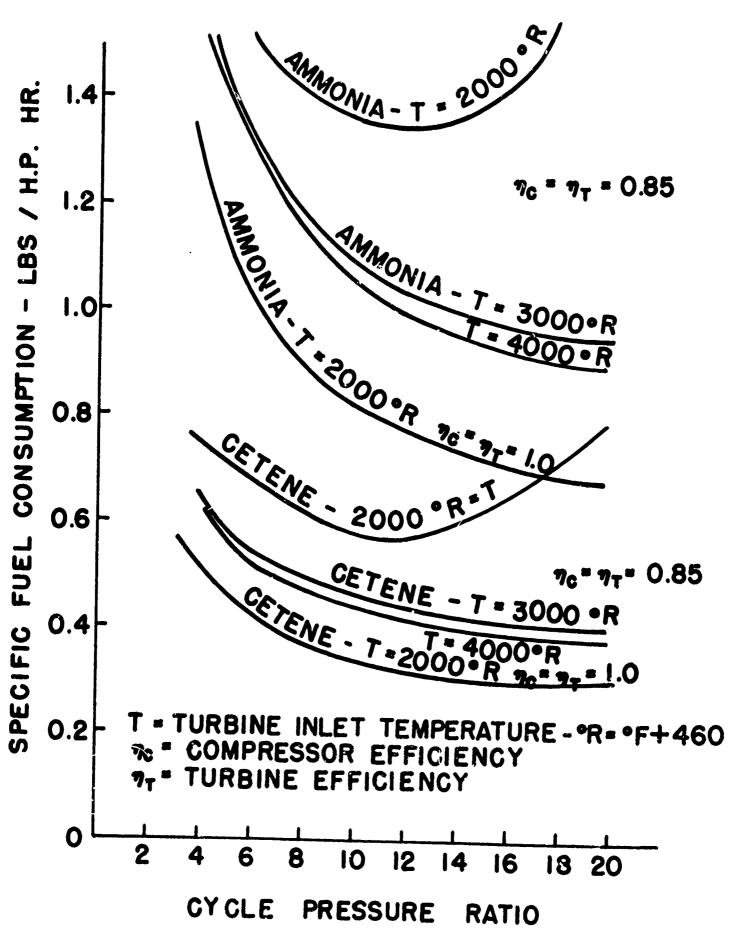


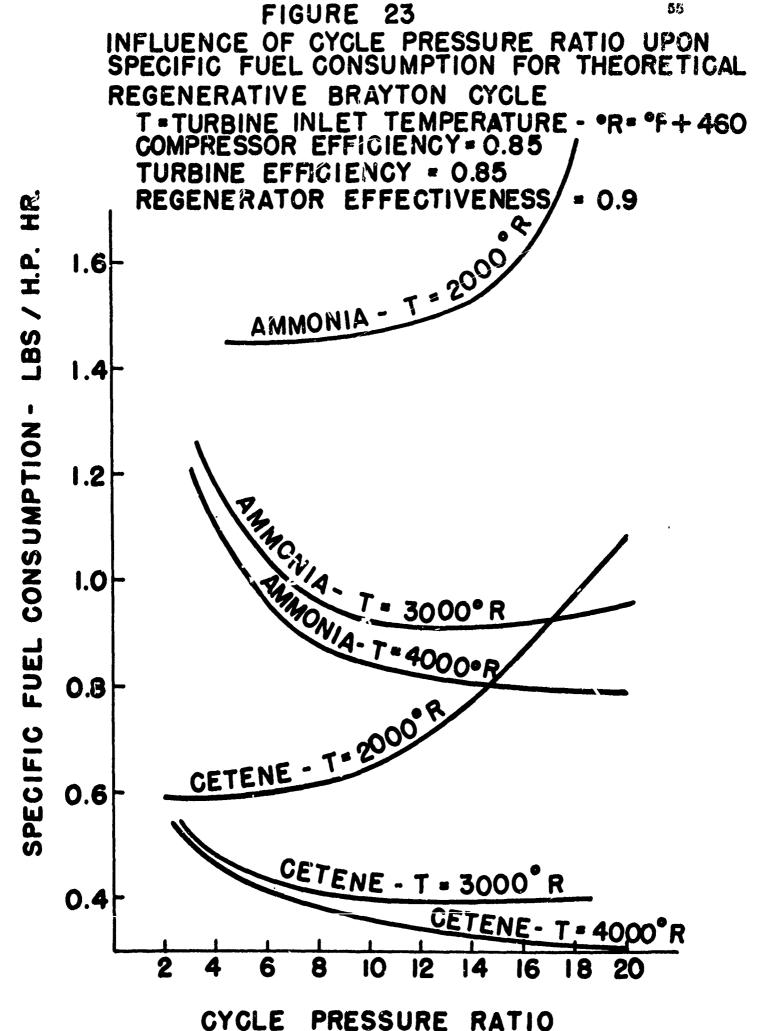
FIGURE 21 53
INFLUENCE OF CYCLE PRESSURE RATIO ON SPECIFIC FUEL CONSUMPTION FOR THEORETICAL NON-REGENERATIVE BRAYTON CYCLE



FIGURE

22

54



APPENDIX

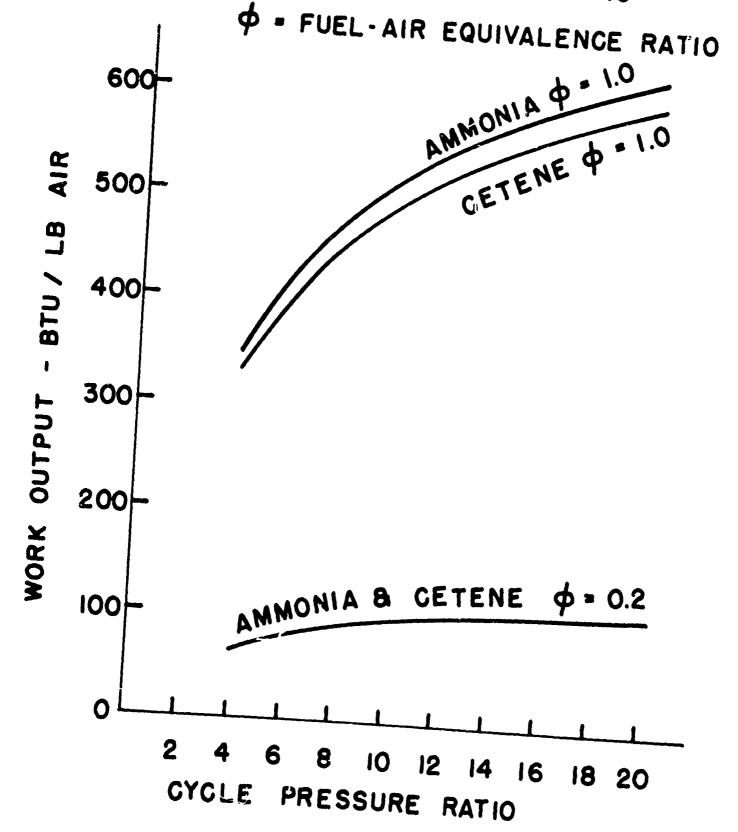
At present the maximum permissible working fluid temperature for turbine operation is limited by material strength considerations. For this reason the results of this report have been presented in terms of peak cycle temperature (or turbine inlet temperature) as a controlling variable.

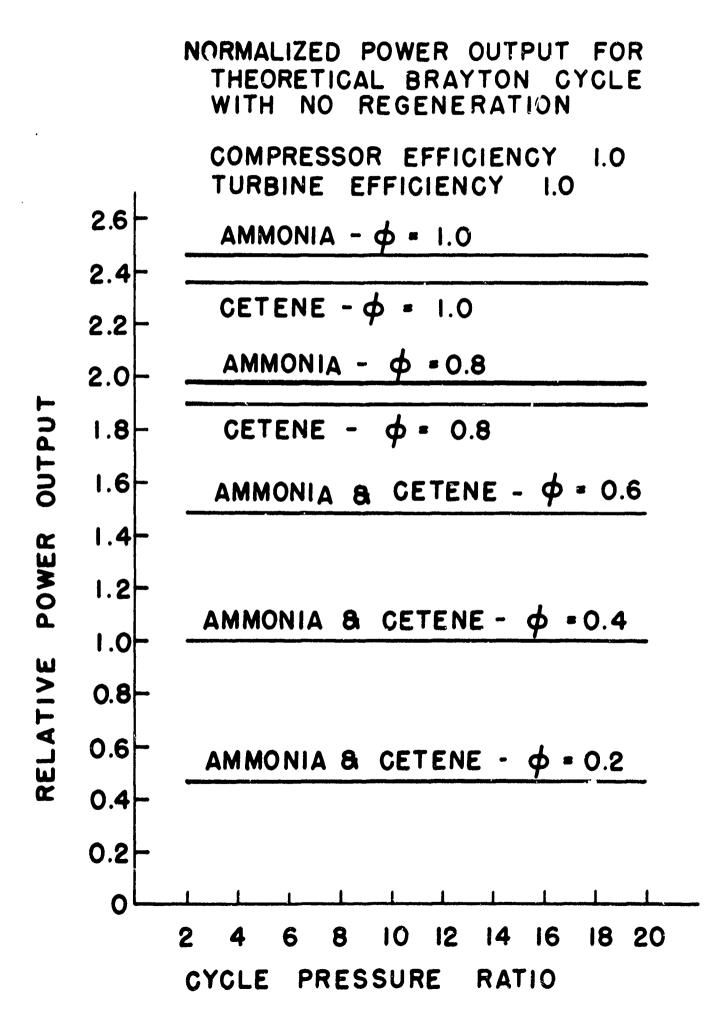
Continued advances in the technology of high temperature materials have progressively increased permissible working fluid temperatures. It is therefore reasonable to expect that at some future time turbine inlet temperature may be of much less significance as a controlling factor.

For this reason, as an appendix to this report, turbine performance has been presented with fuel-to-air equivalence ratio replacing peak cycle temperature as a controlling parameter. The performance features presented in Figures 24 through 39 include power output, thermal efficiency and specific fuel consumption. The independent variables considered are fuel-air equivalence ratio and cycle pressure ratio.

INFLUENCE OF CYCLE PRESSURE RATIO UPON POWER OUTPUT OF THEORETICAL BRAYTON CYCLE WITH NO REGENERATION

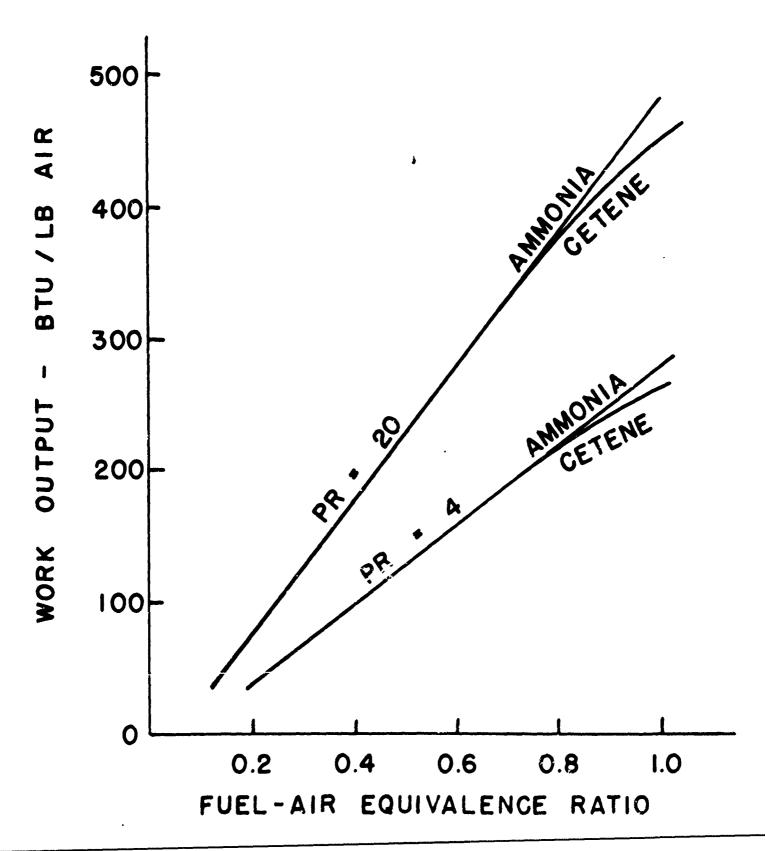
COMPRESSOR EFFICIENCY = 1.0 TURBINE EFFICIENCY = 1.0





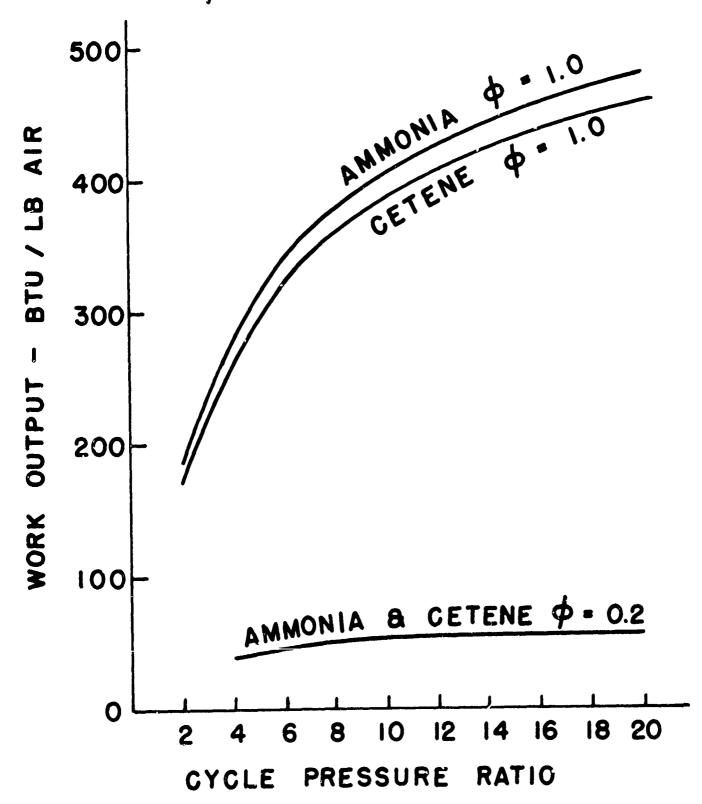
INFLUENCE OF FUEL-AIR RATIO ON POWER OUTPUT OF THEORETICAL BRAYTON CYCLE WITH NO REGENERATION

COMPRESSOR EFFICIENCY - 0.85 TURBINE EFFICIENCY - 0.85



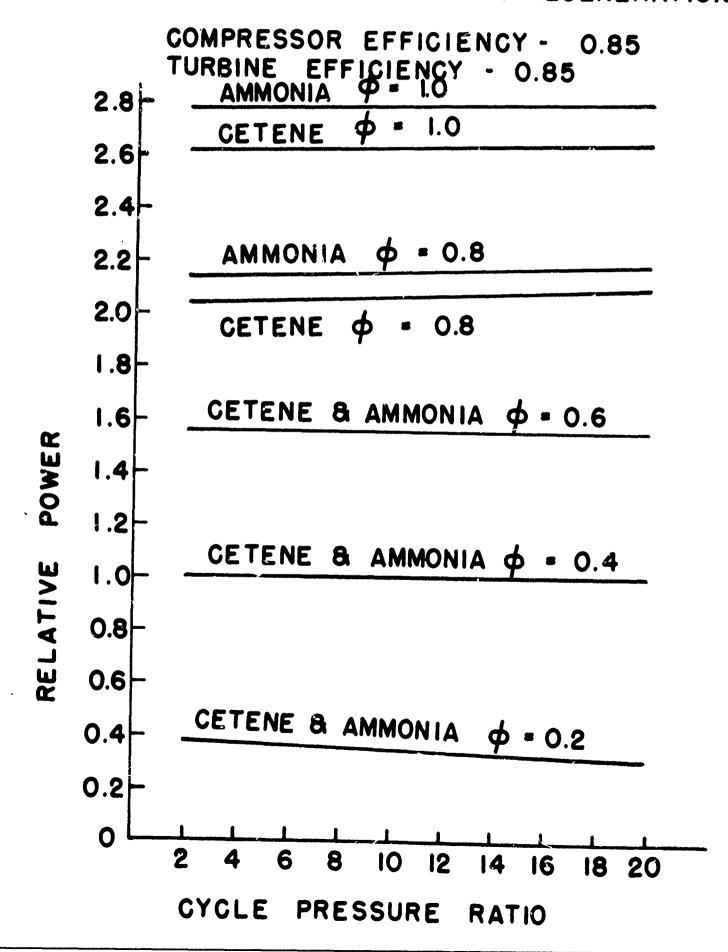
INFLUENCE OF CYCLE PRESSURE RATIO UPON POWER OUTPUT OF THEORETICAL BRAYTON CYCLE WITH NO REGENERATION

COMPRESSOR EFFICIENCY - 0.85 TURBINE EFFICIENCY - 0.85 \$\phi\$ = FUEL-AIR EQUIVALENCE RATIO



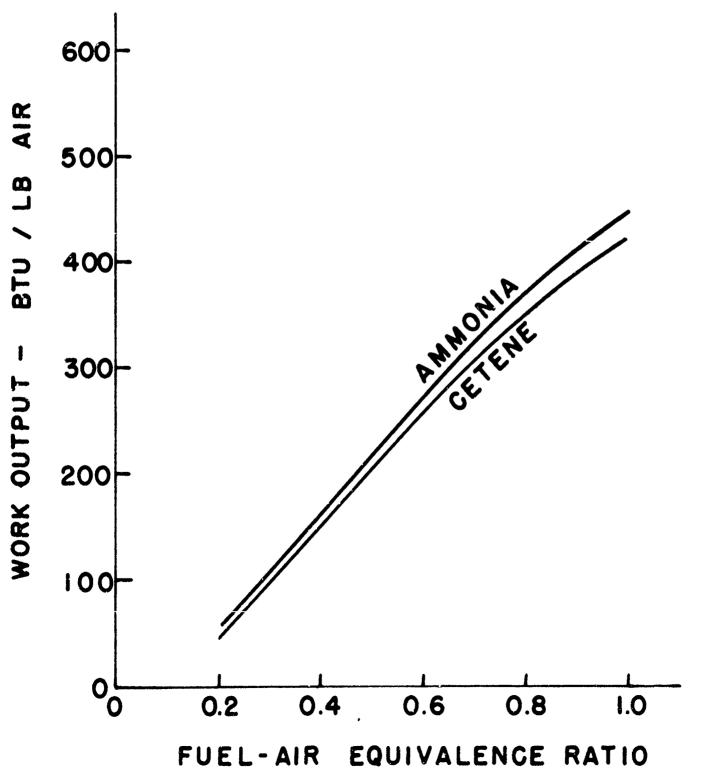
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NORMALIZED POWER OUTPUT FOR THEORETICAL BRAYTON CYCLE WITH NO REGENERATION



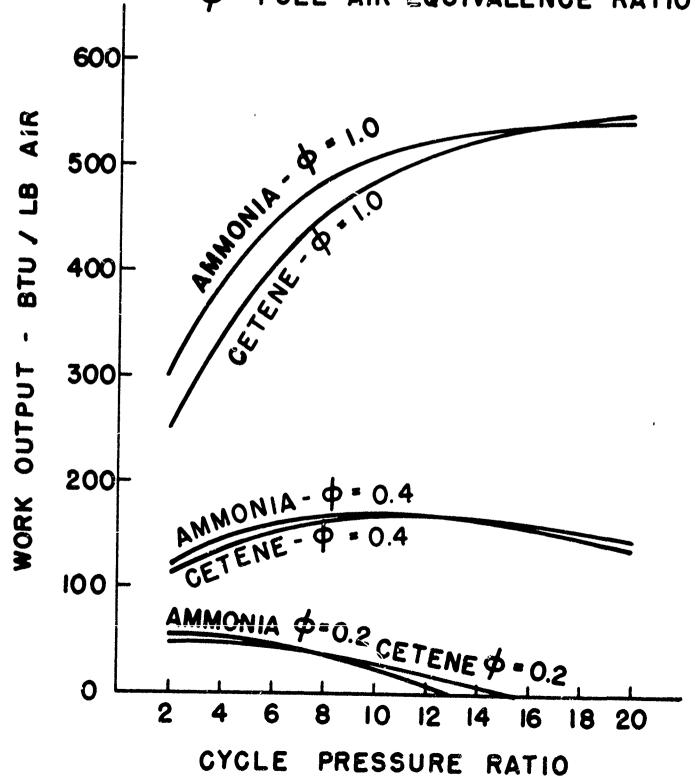
INFLUENCE OF FUEL TO AIR RATIO ON POWER OUTPUT OF THEORETICAL REGENERATIVE BRAYTON CYCLE

CYCLE PRESSURE RATIO - 6 COMPRESSOR EFFICIENCY - 0.85 TURBINE EFFICIENCY - 0.85 REGENERATOR EFFECTIVENESS - 0.9



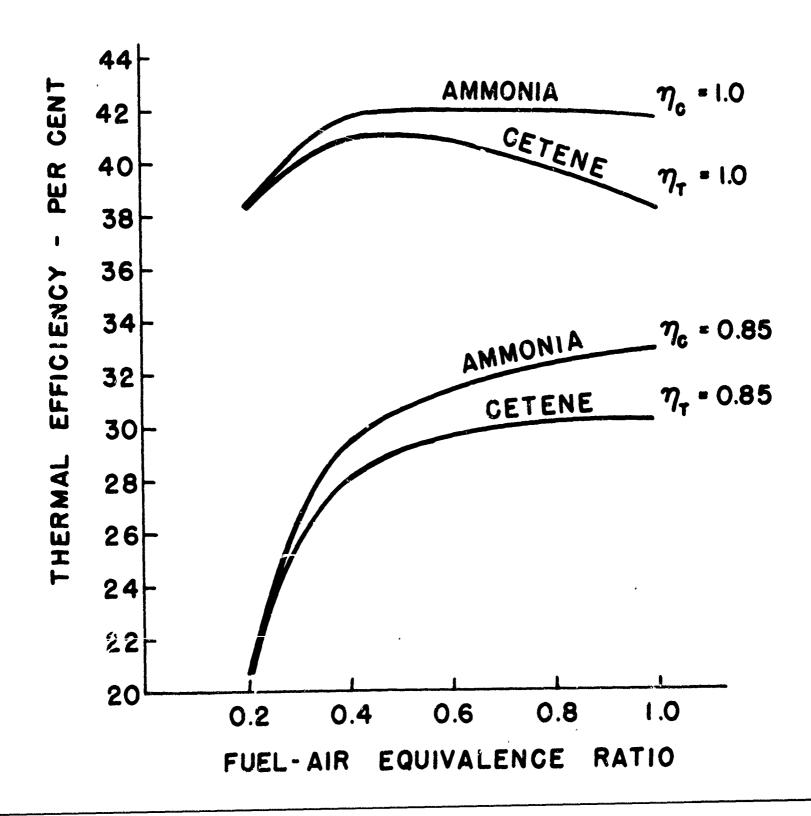
INFLUENCE OF PRESSURE RATIO ON POWER OUTPUT FOR REGENERATIVE BRAYTON CYCLE

COMPRESSOR EFFICIENCY - 0.85
TURBINE EFFICIENCY - 0.85
REGENERATOR EFFECTIVENESS - 0.9
P = FUEL - AIR EQUIVALENCE RATIO

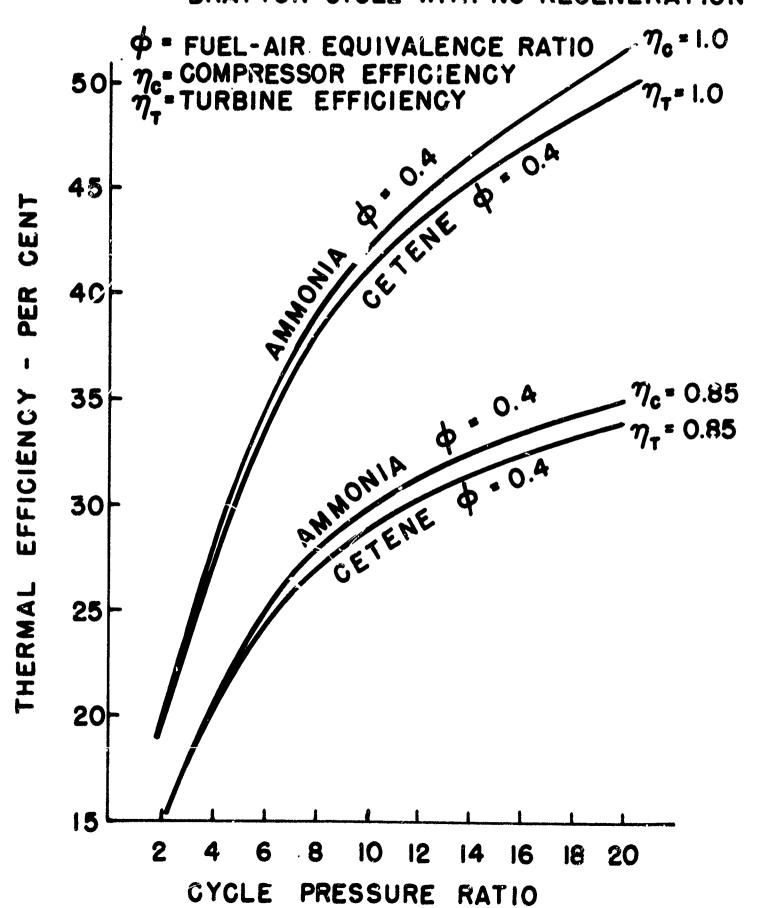


INFLUENCE OF FUEL-AIR RATIO UPON THERMAL EFFICIENCY OF BRAYTON CYCLE WITH NO REGENERATION

CYCLE PRESSURE RATIO = 1.0 η_c = COMPRESSOR EFFICIENCY η_{τ} = TURBINE EFFICIENCY



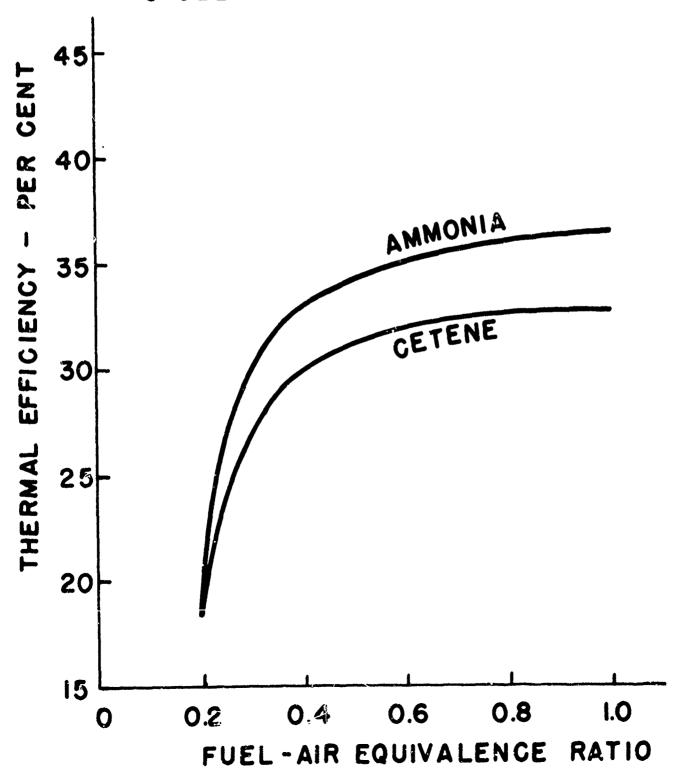
INFLUENCE OF CYCLE PRESSURE RATIO UPON THERMAL EFFICIENCY OF THEORETICAL BRAYTON CYCLE WITH NO REGENERATION



INFLUENCE OF FUEL-AIR RATIO ON THERMAL EFFICIENCY OF THEORETICAL REGENERATIVE BRAYTON CYCLE 1

437

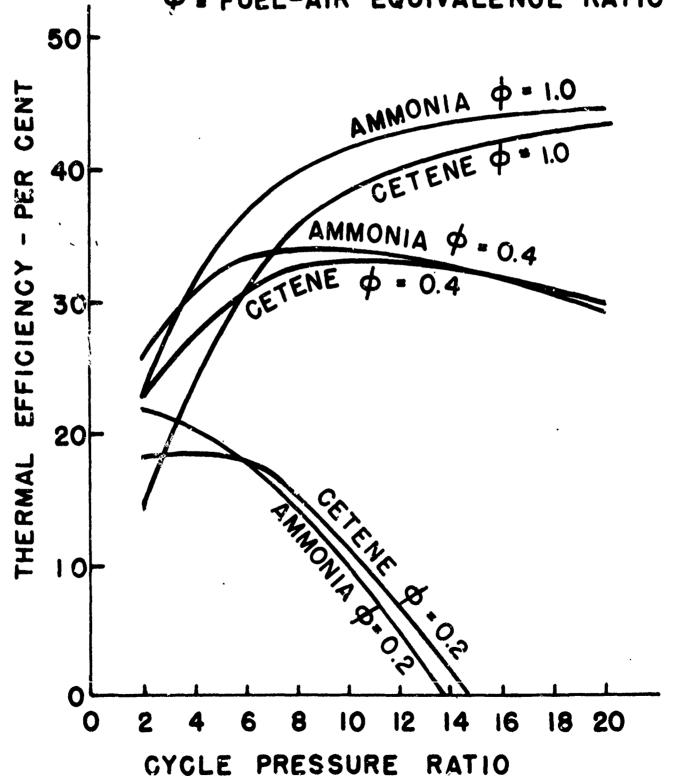
COMPRESSOR EFFICIENCY - 0.85 TURBINE EFFICIENCY - 0.85 REGENERATOR EFFECTIVENESS - 0.9 CYCLE PRESSURE RATIO - 6



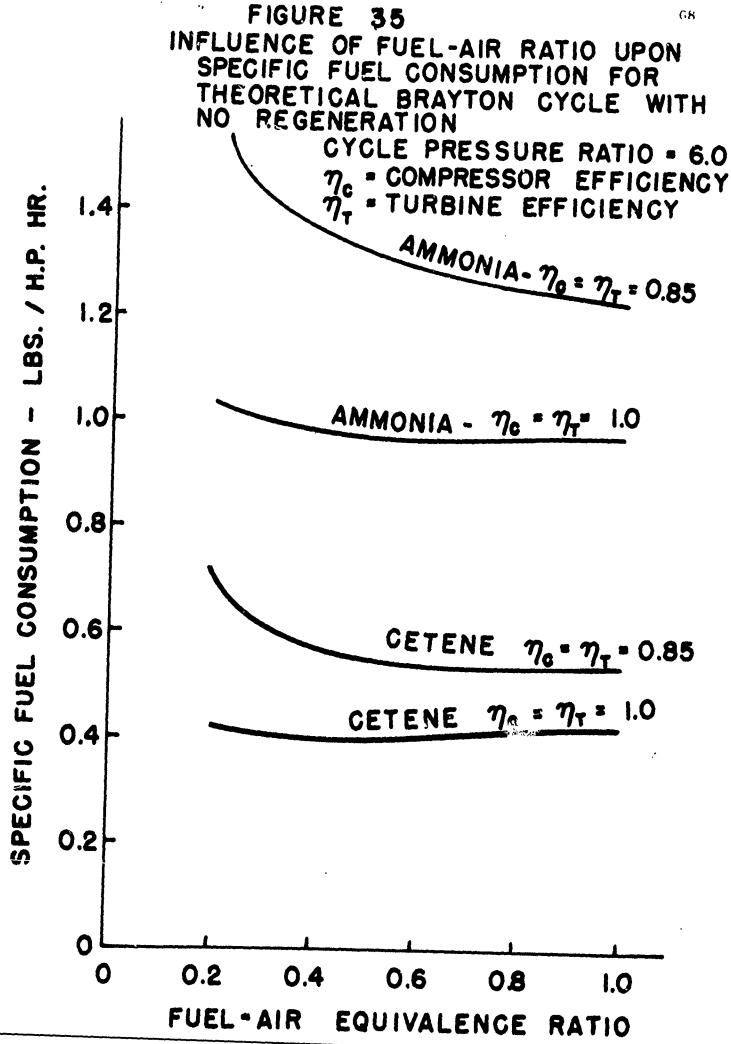
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INFLUENCE OF CYCLE PRESSURE RATIO ON THERMAL EFFICIENCY OF THEORETICAL REGENERATIVE BRAYTON CYCLE

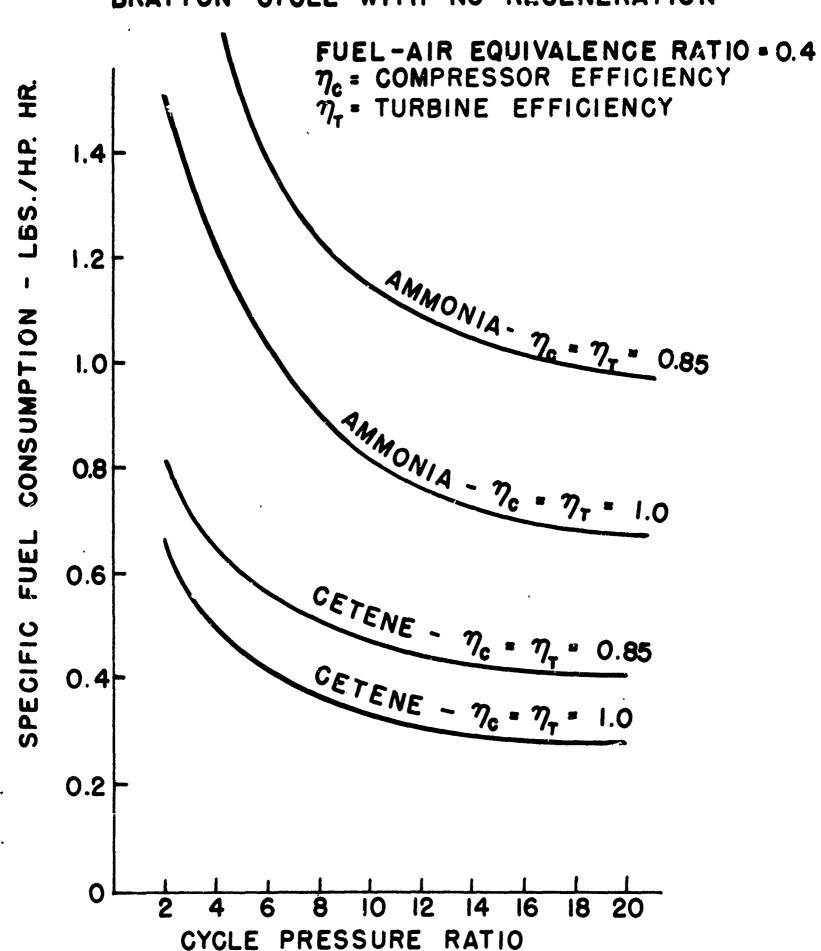
COMPRESSOR EFFICIENCY - 0.85 TURBINE EFFICIENCY - 0.85 REGENERATOR EFFECTIVENESS - 0.9 \$\Phi\$ FUEL-AIR EQUIVALENCE RATIO



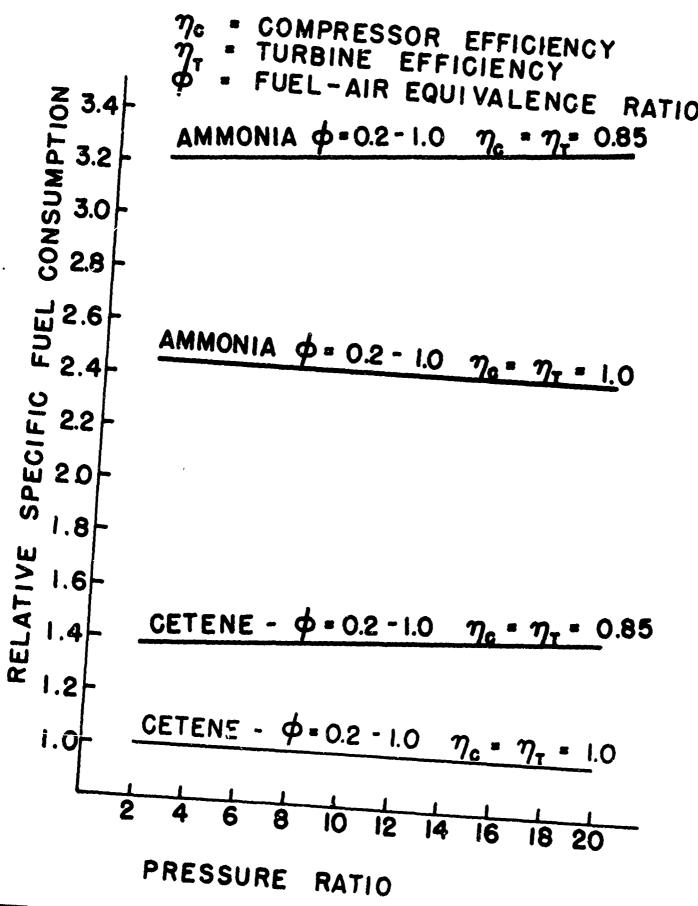




INFLUENCE OF CYCLE PRESSURE RATIO UPON SPECIFIC FUEL CONSUMPTION OF THEORETICAL BRAYTON CYCLE WITH NO REGENERATION



SPECIFIC FUEL CONSUMPTION RELATIVE TO THAT OF CETENE FOR NON-REGENERATIVE BRAYTON CYCLE



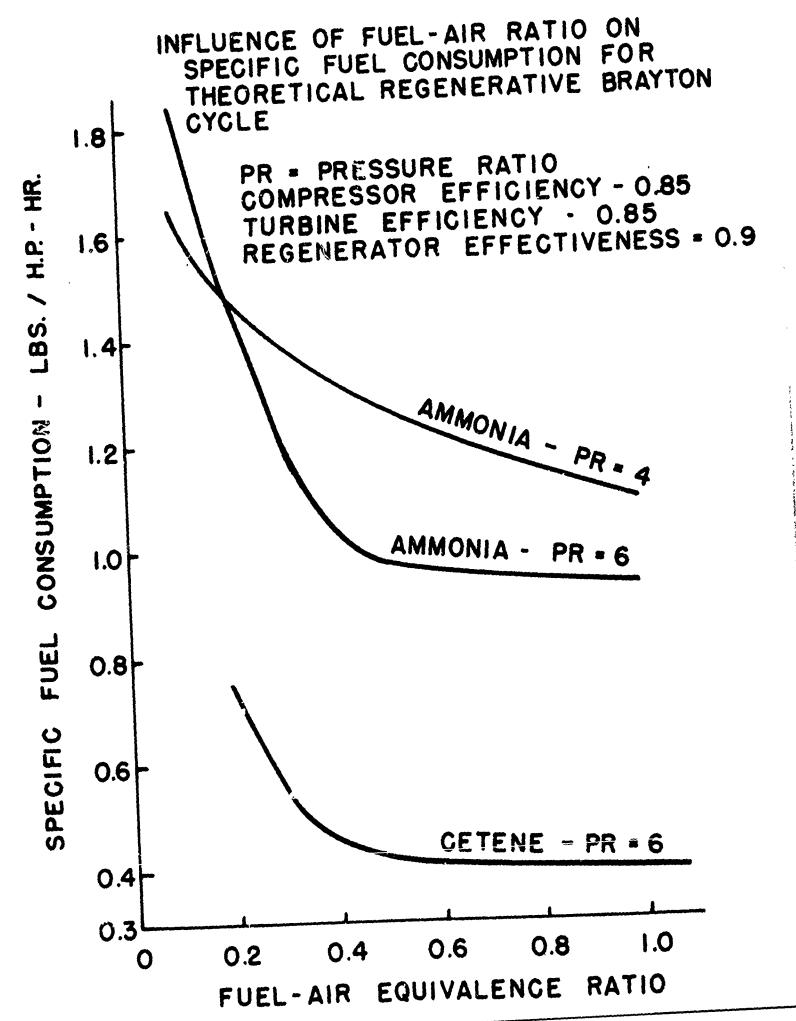


FIGURE 39

INFLUENCE OF CYCLE PRESSURE RATIO ON SPECIFIC FUEL CONSUMPTION FOR THEORETICAL REGENERATIVE BRAYTON CYCLE

